Supporting Information

for

Photolysis of Labile Bonds Towards Radical Generation: Case Study of Alkylverdazyls

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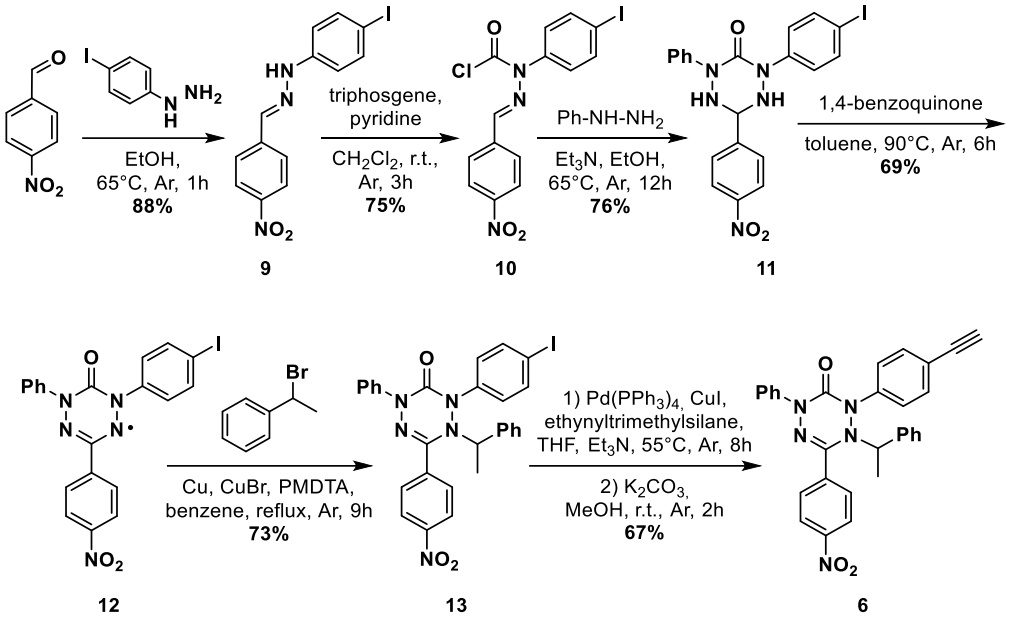
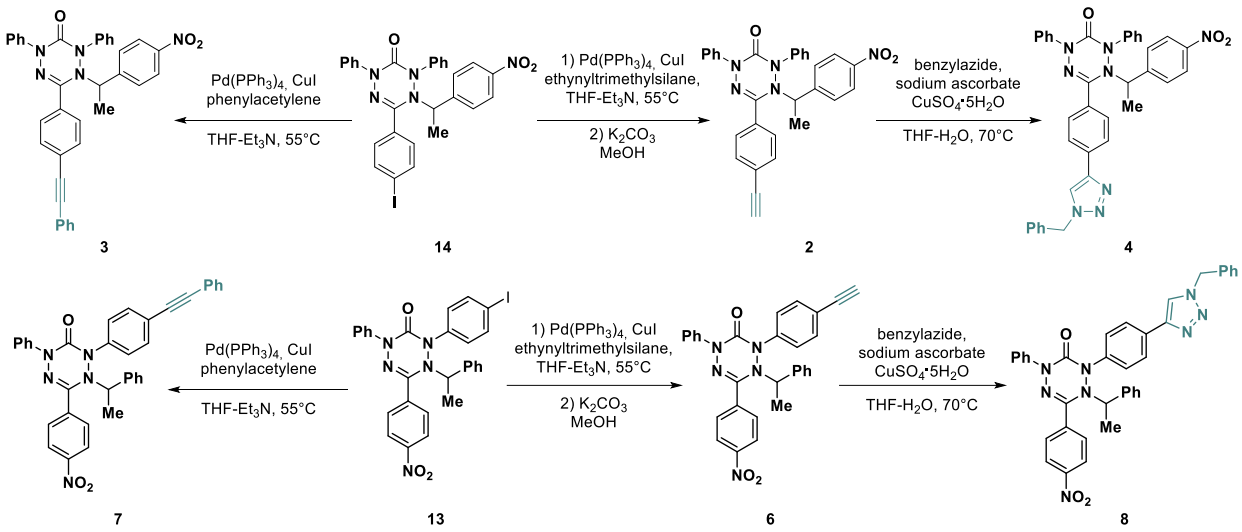
Section S1. Additional Experimental Data



Scheme S1.1. Synthetic path of AlkVZ **6**.



Scheme S1.2. Synthetic paths of AlkVZs **2 – 4** and **6 – 8**.

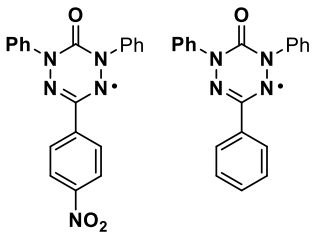


Figure S1.1. Structure of radicals **15** and **16** which were tested for photo-decomposition.

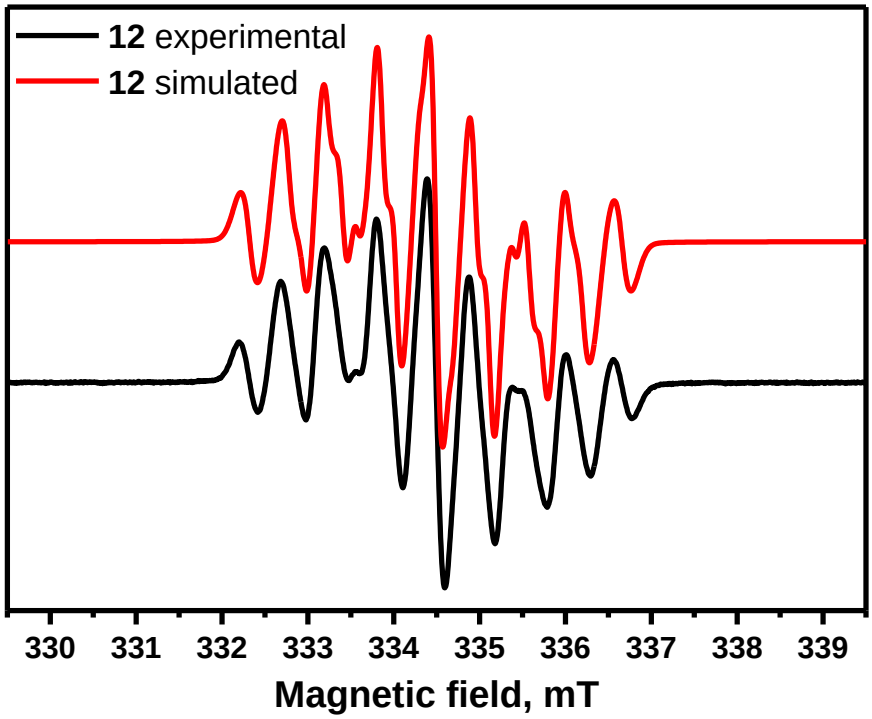


Figure S1.2. Experimental (black) and simulated (red) ESR spectra of radical **12** recorded in deoxygenated toluene solution. Simulation of ESR spectrum was conducted in the Winsim2002 freeware, and hyperfine coupling constants were measured directly from the simulation. [https://www.niehs.nih.gov/research/resources/software/tox-pharm/tools]

Section S2. Measurement of AlkVZs 1 – 8 rate constants and quantum yield calculation

General

Competitive first order reaction equation:

$[radical]/[AlkVZ]_0 = \frac{k_1}{k_1+k_2}\left(1 - e^{-(k_1+k_2)t}\right)$

Negative first order reaction equation:

$[radical] = \sqrt{[AlkVZ]_0^2 - 2k_3 \cdot t}$

Negative second order equation:

$[radical] = \sqrt[3]{[AlkVZ]_0^3 - 3k_3 \cdot t}$

k_1 – rate constant for homolysis, s^{-1};
k_2 – rate constant for side reaction, s^{-1};
k_3 – rate constant for verdazyl radical degradation;
[radical] – concentration of verdazyl radical at time moment t, M;
$[AlkVZ]_0$ – initial concentration of alkylverdazyl, M;
t – reaction time, s.

Integral quantum yields (Φ) at time (t) were calculated according to the following equation:

$$\Phi = \frac{C_0 \cdot V \cdot N_A \cdot Y}{N_p \cdot (1 - 10^{-\varepsilon C_0 l})}$$

C_0 – initial concentration of alkylverdazyl, M;
V – sample volume, L;
N_A – the Avogadro constant;
Y – yield of radical at the time t;
ε – molar extinction coefficient, $cm^{-1} \cdot M^{-1}$;
l – path length of irradiation, cm (taken as 0.3 cm).

AlkVZ 1

Table S2.1. Data for photolysis of AlkVZ **1** using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00831	0.01127	0.00751	0.00903	0.00198
5	0.30483	0.31692	0.32715	0.31630	0.01117
10	0.55125	0.60456	0.53809	0.56463	0.03520
20	0.69305	0.73223	0.68341	0.70290	0.02586
30	0.72165	0.75176	0.73467	0.73603	0.01510
60	0.72498	0.72096	0.72209	0.72268	0.00207

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

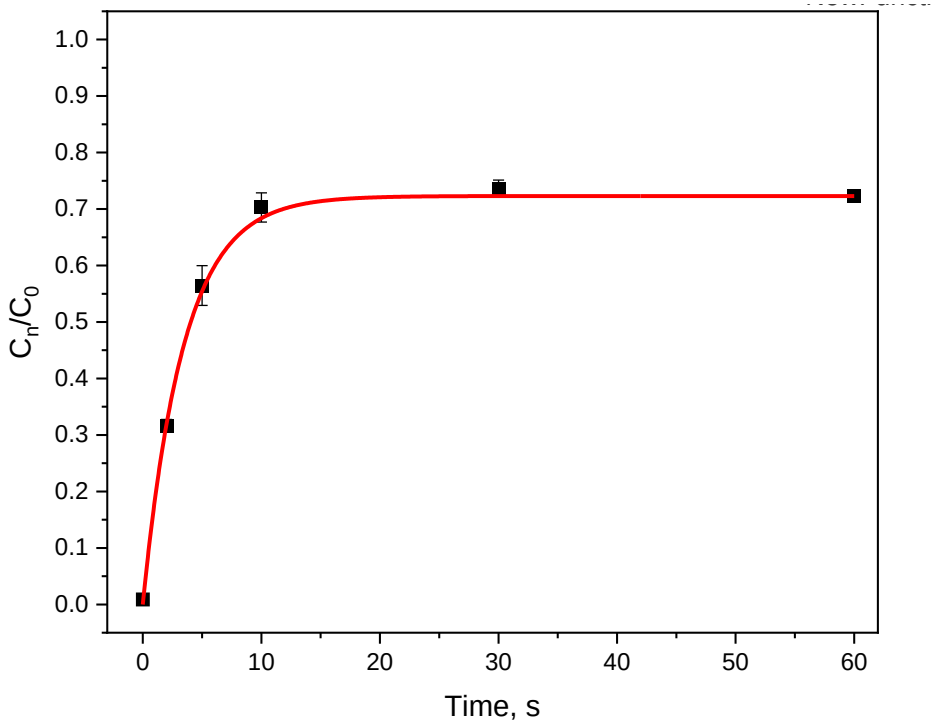


Figure S2.1. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **1** using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99956; k_1=2.105E-1 s^{-1} (standard error 2.201E-2 s^{-1}); k_2=8.065E-2 s^{-1} (standard error 8.710E-3 s^{-1}).

Table S2.2. Data for photolysis of AlkVZ **1** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.01109	0.01091	0.01091	0.01097	0.00010
5	0.14799	0.13322	0.13922	0.14014	0.00743
10	0.26176	0.25863	0.26616	0.26218	0.00378
20	0.43380	0.42966	0.43075	0.43140	0.00215
30	0.55732	0.54053	0.54464	0.54750	0.00875
60	0.69635	0.65794	0.67103	0.67511	0.01953
90	0.73928	0.70738	0.70447	0.71704	0.01931
120	0.74889	0.73086	0.72744	0.73573	0.01152
180	0.77034	0.73028	0.73046	0.74369	0.02308
300	0.77663	0.73319	0.72214	0.74399	0.02880

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

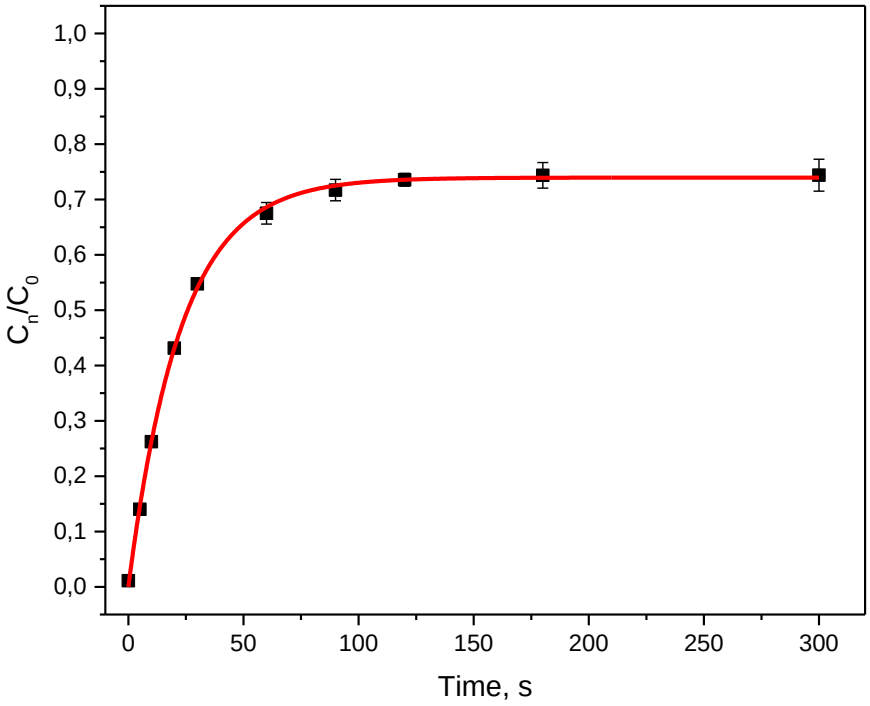


Figure S2.2. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **1** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99676; k_1=3.238E-2 s^{-1} (standard error 1.220E-3 s^{-1}); k_2=1.140E-2 s^{-1} (standard error 2.270E-3 s^{-1}).

Table S2.3. Data for photolysis of AlkVZ **1** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.01360	0.00773	0.01538	0.01224	0.00400
30	0.04004	0.03867	0.04168	0.04013	0.00151
60	0.07369	0.06264	0.06903	0.06845	0.00555
120	0.13284	0.11175	0.14643	0.13034	0.01747
300	0.25515	0.24592	0.24964	0.25024	0.00464
600	0.41764	0.41865	0.42068	0.41899	0.00155
1200	0.59415	0.58580	0.57857	0.58617	0.00780
1800	0.69084	0.67416	0.68901	0.68467	0.00915
2700	0.75297	0.72423	0.73053	0.73591	0.01511
3600	0.76959	0.77334	0.76408	0.76900	0.00466
4500	0.77809	0.75497	0.75964	0.76423	0.01223

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

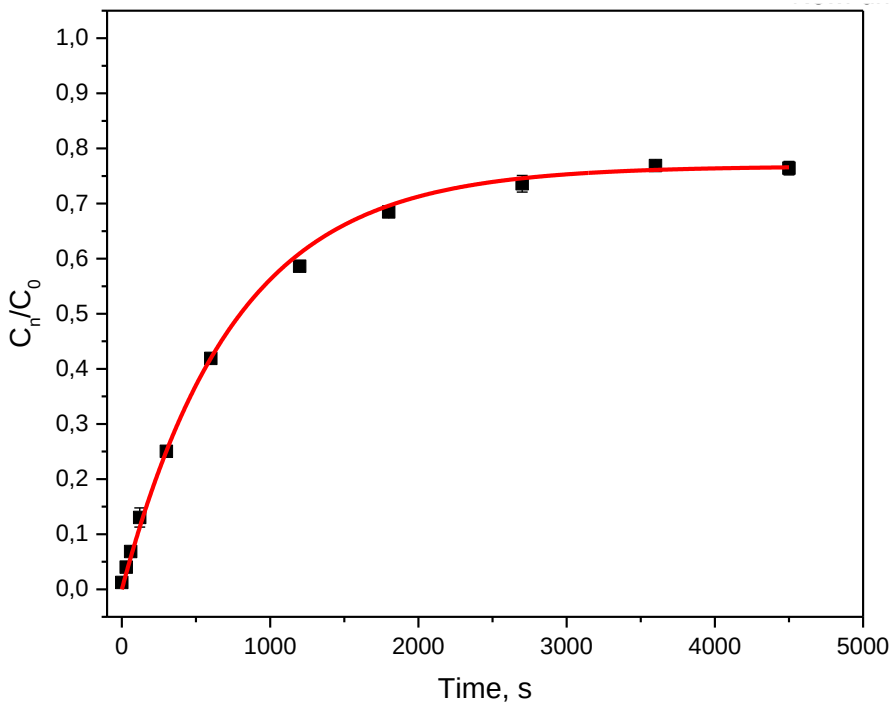


Figure S2.3. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **1** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99849; k_1=1.01E-3 s^{-1} (standard error 1.827E-5 s^{-1}); k_2=3.058E-4 s^{-1} (standard error 2.461E-5 s^{-1}).

Table S2.4. Data for photolysis of AlkVZ **1** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00659	0.00958	0.00635	0.00751	0.00180
30	0.05927	0.06070	0.05679	0.05892	0.00198
60	0.11037	0.11642	0.10883	0.11187	0.00401
90	0.16717	0.17230	0.16381	0.16776	0.00428
120	0.19756	0.21760	0.21181	0.20899	0.01031
180	0.28337	0.30518	0.27429	0.28761	0.01588
240	0.34870	0.36192	0.34987	0.35350	0.00732
300	0.40639	0.41415	0.39695	0.40583	0.00861
360	0.44946	0.44879	0.44483	0.44769	0.00250
450	0.48920	0.49403	0.50730	0.49684	0.00937
600	0.55400	0.57300	0.56968	0.56556	0.01015
750	0.58979	0.58843	0.60044	0.59289	0.00658
900	0.62242	0.59393	0.62041	0.61225	0.01590
1200	0.64656	0.63169	0.65371	0.64399	0.01123
1500	0.67046	0.64703	0.67654	0.66468	0.01558
1800	0.66447	0.63898	0.67222	0.65856	0.01739
2400	0.65591	0.64073	0.66737	0.65467	0.01336

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

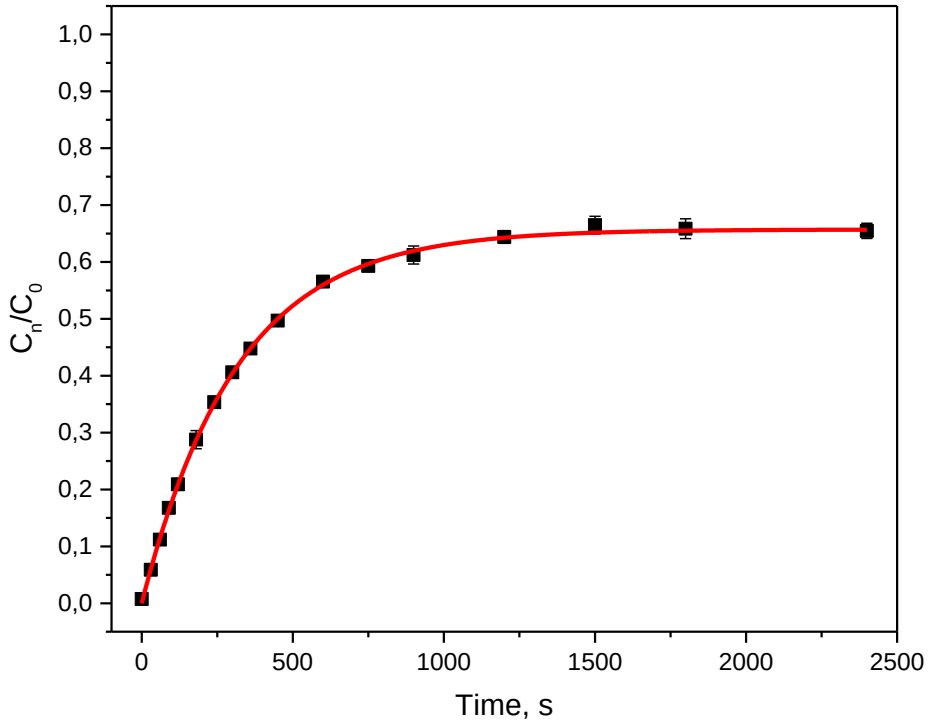


Figure S2.4. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **1** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.99941; k_1=2.090E-3 s^{-1} (standard error 2.682E-5 s^{-1}); k_2= 1.090 s^{-1} (standard error 4,359E-5 s^{-1}).

AlkVZ 5

Table S2.5. Data for photolysis of AlkVZ **5** using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.22920	0.23942	0.23268	0.23377	0.00520
10	0.45066	0.43577	0.43996	0.44213	0.00768
20	0.65876	0.62165	0.65530	0.64524	0.02050
30	0.73321	0.72719	0.74542	0.73527	0.00929
60	0.76277	0.75365	0.78815	0.76819	0.01788
120	0.72263	0.70073	0.72460	0.71599	0.01325

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

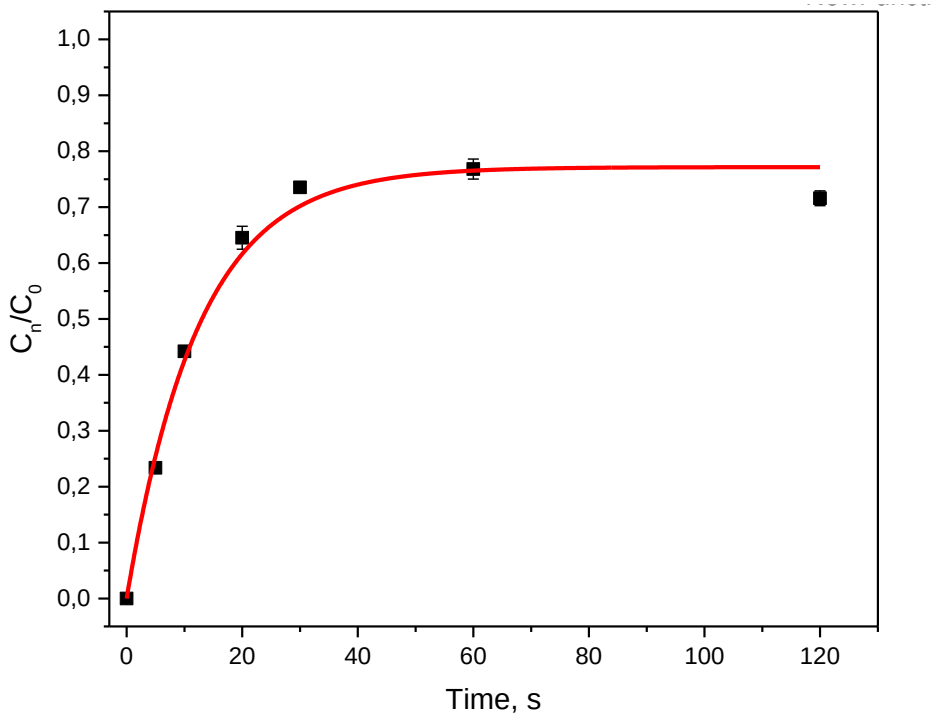


Figure S2.5. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99607; k_1=6.183E-2 s^{-1} (standard error 3.870E-3 s^{-1}); k_2=1.830E-2 s^{-1} (standard error 3.680E-3 s^{-1}).

Table S2.6. Data for photolysis of AlkVZ **5** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.20399	0.14370	0.16507	0.17092	0.03057
10	0.36932	0.30241	0.33415	0.33529	0.03347
20	0.53353	0.50093	0.52661	0.52036	0.01718
30	0.65841	0.61666	0.65600	0.64369	0.02344
45	0.73235	0.74100	0.75450	0.74262	0.01116
60	0.81963	0.77556	0.79750	0.79756	0.02204
90	0.82957	0.80185	0.81349	0.81497	0.01392
120	0.84399	0.85089	0.82970	0.84153	0.01081
180	0.80591	0.80556	0.79220	0.80122	0.00782

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

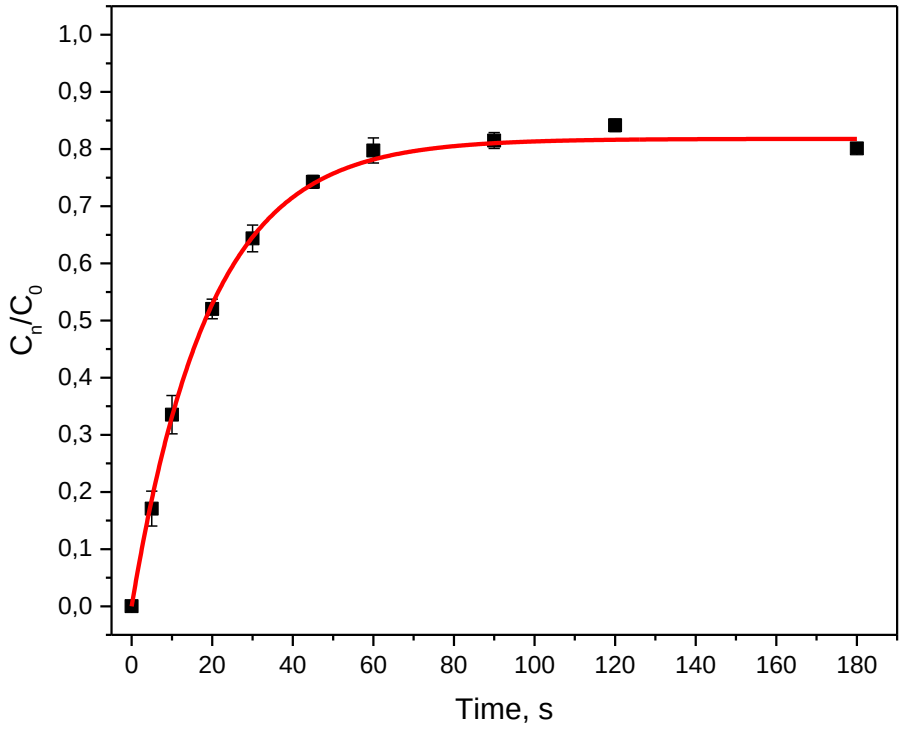


Figure S2.6. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99952; k_1=4.252E-2 s^{-1} (standard error 1.890E-3 s^{-1}); k_2=9.47E-3 s^{-1} (standard error 7.062E-4 s^{-1}).

Table S2.7. Data for photolysis of AlkVZ **5** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.09429	0.11853	0.09368	0.10217	0.01417
30	0.27917	0.32311	0.26218	0.28815	0.03144
60	0.47854	0.50279	0.43081	0.47071	0.03662
120	0.64167	0.68833	0.63935	0.65645	0.02763
180	0.73796	0.78167	0.72909	0.74957	0.02815
300	0.76738	0.81382	0.78712	0.78944	0.02331
420	0.76833	0.82869	0.80282	0.79995	0.03028
600	0.77083	0.81777	0.78285	0.79048	0.02438

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

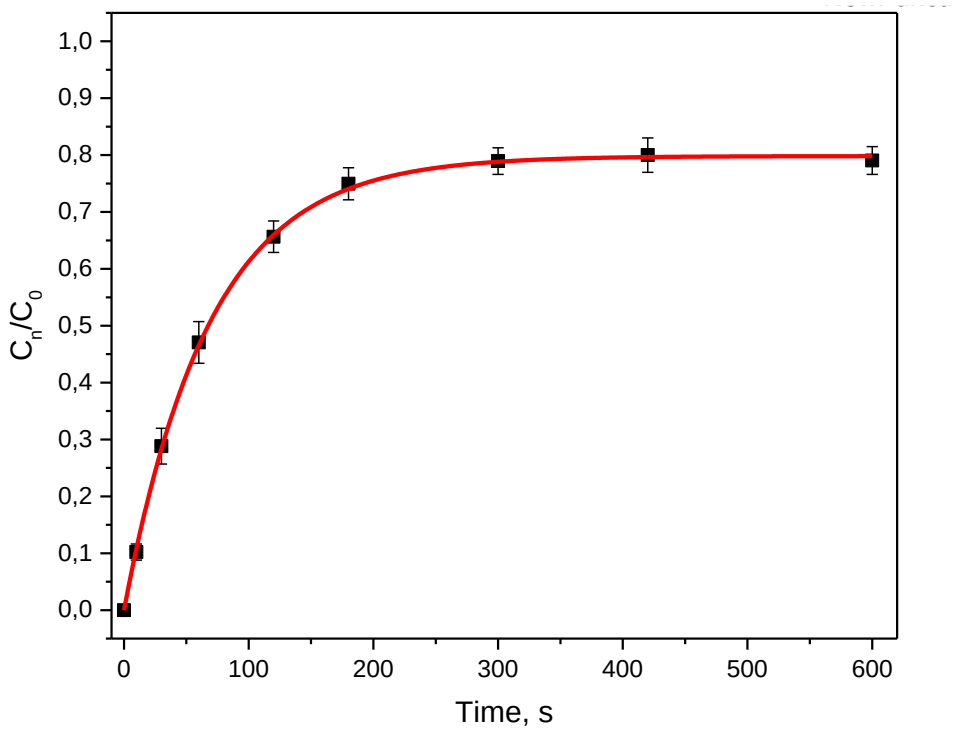


Figure S2.7. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99988; k_1=1.165E-2 s^{-1} (standard error 1.970E-4 s^{-1}); k_2=2.940E-3 s^{-1} (standard error 9.962E-5 s^{-1}).

Table S2.8. Data for photolysis of AlkVZ **5** using 530 nm LED (58 mW power, $1.562 \cdot 10^{17}$ photons per second photons per second).

Time, s	Y
0	0
1800	0.0244
3600	0.04583
7200	0.06182
10800	0.08017
14400	0.08831
18000	0.10172
21600	0.11985
25200	0.12331
28800	0.12677
32400	0.13875
36000	0.14073
39600	0.14914
43200	0.15595
46800	0.15848
54000	0.15441

Y– experimental yield of radical determined via EPR spectroscopy.

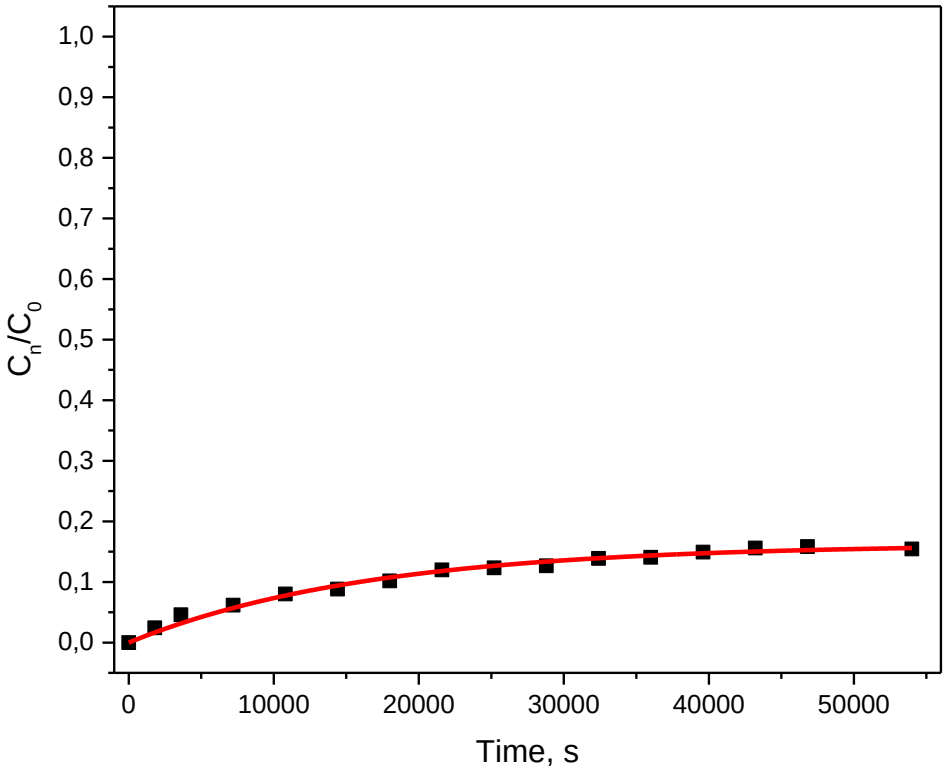


Figure S2.8. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 530 nm LED (58 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.98555; k_1=9.772E-6 s^{-1} (standard error 5.234E-7 s^{-1}); k_2=5.043E-5 s^{-1} (standard error 4.173E-6 s^{-1}).

Table S2.9. Data for photolysis of AlkVZ **5** using 367 nm LED (7.00 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00000	0.00000	0.00000	0.00000	0.00000
15	0.10660	0.08013	0.11528	0.10067	0.01831
30	0.18409	0.15855	0.16536	0.16933	0.01323
60	0.34626	0.27740	0.29889	0.30752	0.03523
120	0.46230	0.47357	0.40596	0.44728	0.03622
180	0.56409	0.51791	0.50238	0.52813	0.03210
300	0.66132	0.64817	0.70800	0.67250	0.03144
450	0.70677	0.70060	0.67191	0.69309	0.01860
600	0.72766	0.71672	0.71421	0.71953	0.00715
900	0.68991	0.70532	0.66753	0.68759	0.01900

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

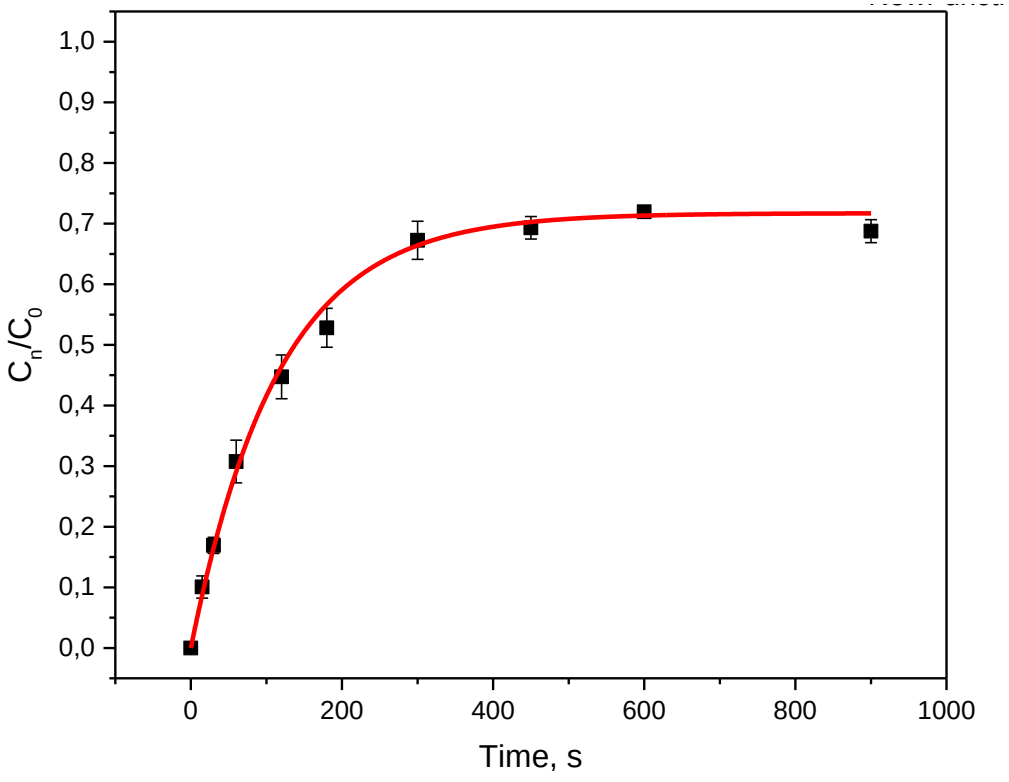


Figure S2.9. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 367 nm LED (7.00 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99943; k_1=6.220E-3 s^{-1} (standard error 3.418E-4 s^{-1}); k_2=2.450E-3 s^{-1} (standard error 1.738E-4 s^{-1}).

Table S2.10. Data for photolysis of AlkVZ **5** using 382 nm LED (6.70 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00000	0.00000	0.00000	0.00000	0.00000
30	0.15026	0.14540	0.14319	0.14628	0.00362
60	0.23391	0.23804	0.26306	0.24500	0.01577
120	0.45238	0.37843	0.36502	0.39861	0.04705
180	0.57323	0.58055	0.56932	0.57437	0.00570
300	0.61391	0.70711	0.60055	0.64052	0.05805
450	0.78706	0.79064	0.64787	0.74186	0.08141
600	0.80264	0.79055	0.80187	0.79835	0.00677
900	0.69872	0.75323	0.77502	0.74232	0.03930

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

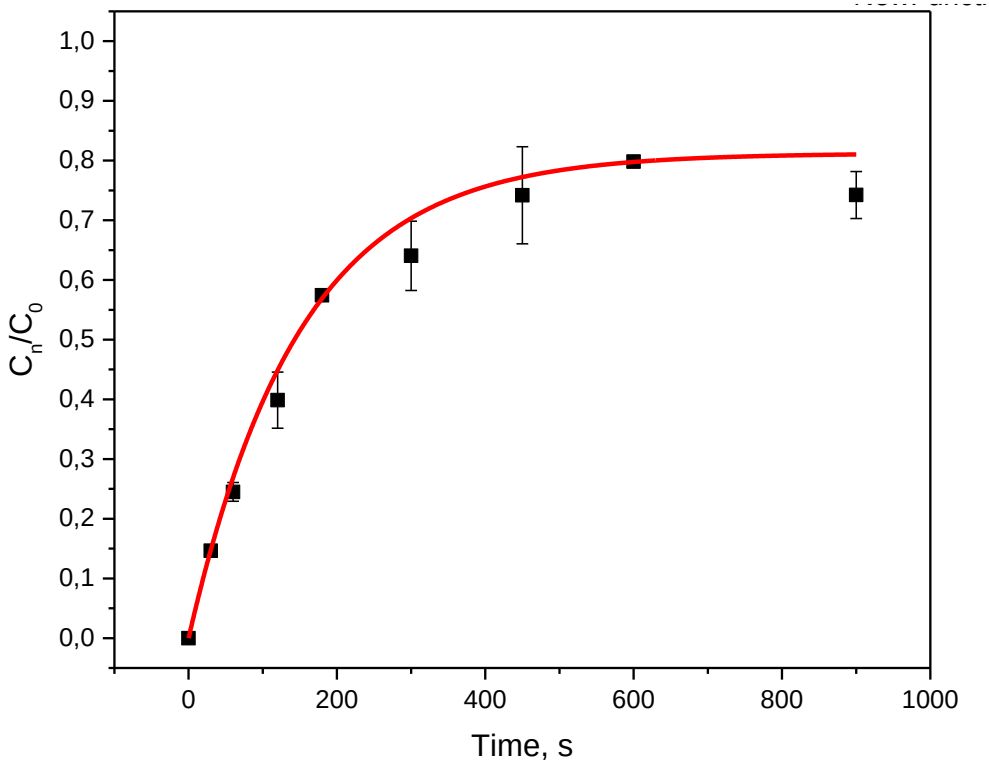


Figure S2.10. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 382 nm LED (6.70 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99958; k_1=5.440E-3 s^{-1} (standard error 1.104E-4 s^{-1}); k_2=1.260E-3 s^{-1} (standard error 8.802E-5 s^{-1}).

Table S2.11. Data for photolysis of AlkVZ **5** using 392 nm LED (6.53 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.03265	0.00053	0.00463	0.01260	0.01748
30	0.15820	0.13073	0.10131	0.13008	0.02845
60	0.30686	0.23257	0.20527	0.24823	0.05258
120	0.38992	0.38678	0.41959	0.39876	0.01810
180	0.48980	0.51445	0.54065	0.51497	0.02543
300	0.70453	0.63327	0.65702	0.66494	0.03628
450	0.76122	0.69706	0.71384	0.72404	0.03327
600	0.78453	0.71400	0.61286	0.70380	0.08629
900	0.76110	0.70624	0.75033	0.73922	0.02907
1200	0.76392	0.70147	0.73604	0.73381	0.03128

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

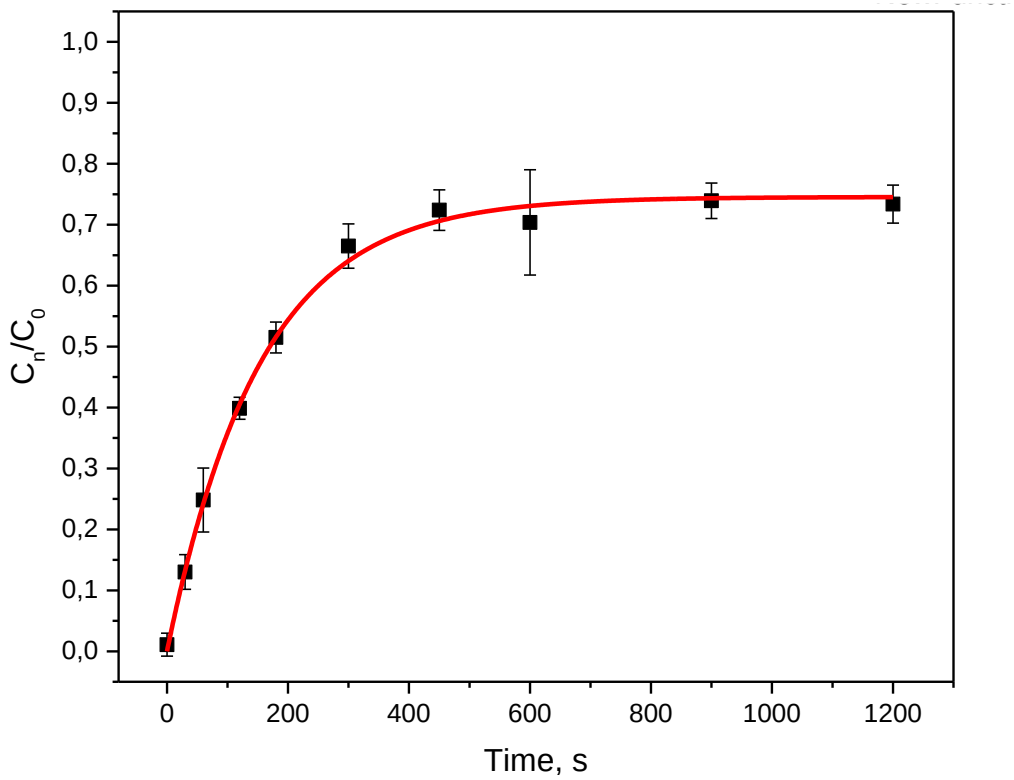


Figure S2.11. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 392 nm LED (6.53 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99826; k_1=4.870E-3 s^{-1} (standard error 1.145E-4 s^{-1}); k_2=1.660E-3 s^{-1} (standard error 9.494E-5 s^{-1}).

Table S2.12. Data for photolysis of AlkVZ **5** using 405 nm LED (6.32 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.02511	0.03149	0.02000	0.02553	0.00576
30	0.12060	0.14681	0.10843	0.12528	0.01961
60	0.24396	0.23970	0.21552	0.23306	0.01534
120	0.33004	0.32928	0.33561	0.33164	0.00346
180	0.42051	0.49970	0.38217	0.43413	0.05994
300	0.62557	0.64060	0.58626	0.61748	0.02806
450	0.72340	0.74034	0.69087	0.71820	0.02514
600	0.75970	0.73447	0.73500	0.74306	0.01442
900	0.77745	0.80187	0.75287	0.77740	0.02450
1200	0.77123	0.79438	0.75404	0.77322	0.02024
1800	0.74783	0.76613	0.75354	0.75583	0.00936

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

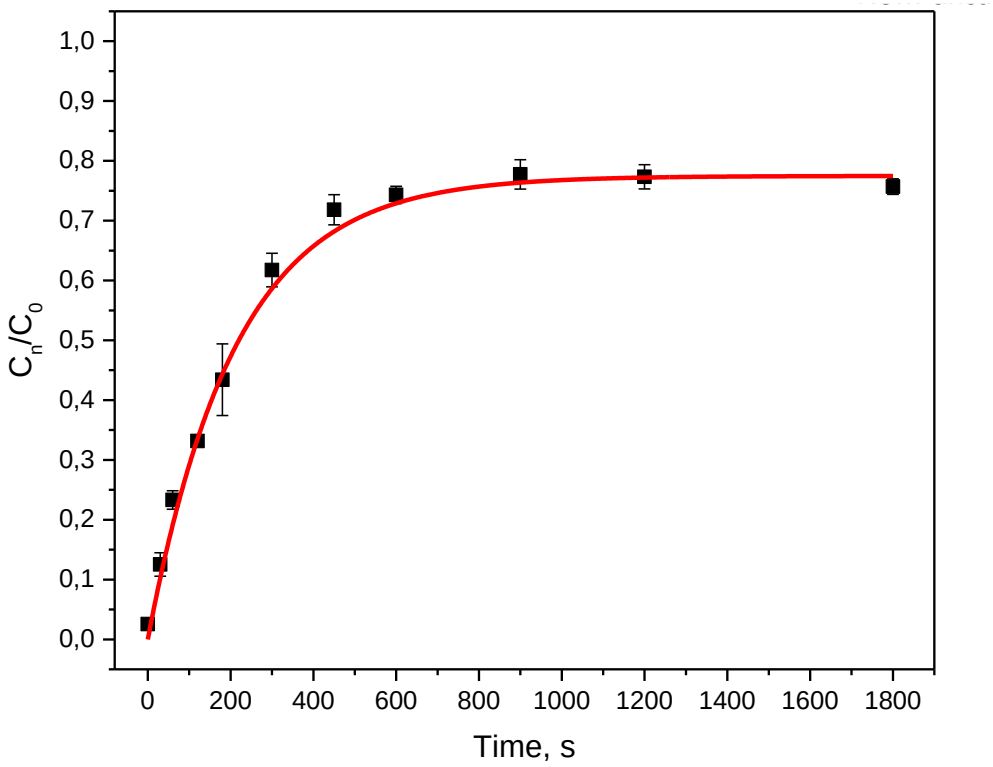


Figure S2.12. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 405 nm LED (6.32 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99332; k_1=3.650E-3 s^{-1} (standard error 1.050E-4 s^{-1}); k_2=1.060E-3 s^{-1} (standard error 1.231E-4 s^{-1}).

Table S2.13. Data for photolysis of AlkVZ **5** using 415 nm LED (6.17 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.03200	0.03289	0.02044	0.02844	0.00695
30	0.09342	0.08831	0.09124	0.09099	0.00256
60	0.16222	0.14209	0.12253	0.14228	0.01985
120	0.26827	0.27164	0.27187	0.27059	0.00202
180	0.36587	0.37289	0.36636	0.36837	0.00392
300	0.49644	0.51058	0.49716	0.50139	0.00796
450	0.58622	0.50902	0.49471	0.52998	0.04923
600	0.63484	0.69387	0.66236	0.66369	0.02954
900	0.67493	0.73840	0.71636	0.70990	0.03222
1200	0.70009	0.74813	0.72871	0.72564	0.02417
1800	0.68769	0.75867	0.73707	0.72781	0.03638

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

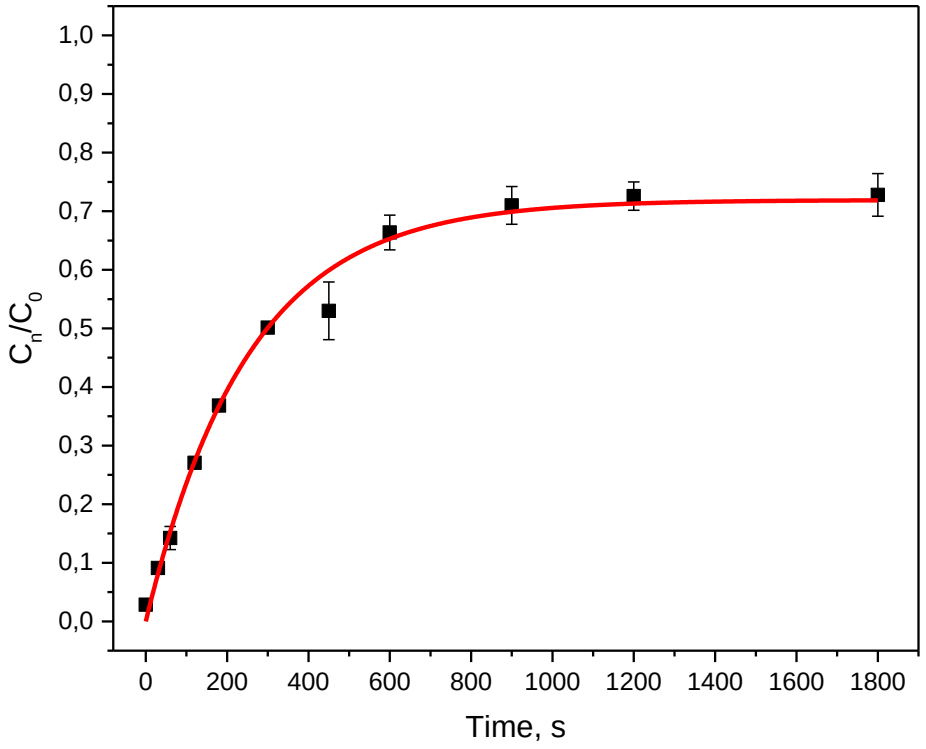


Figure S2.13. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 415 nm LED (6.17 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99473; k_1=2.860E-3 s^{-1} (standard error 6.184E-5 s^{-1}); k_2=1.120E-3 s^{-1} (standard error 1.849E-4 s^{-1}).

Table S2.14. Data for photolysis of AlkVZ **5** using 425 nm LED (6.02 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.02936	0.02851	0.03244	0.03010	0.00207
60	0.12340	0.11064	0.10844	0.11416	0.00808
120	0.17821	0.17855	0.19049	0.18242	0.00699
180	0.29732	0.25957	0.22222	0.25970	0.03755
300	0.37277	0.38826	0.38582	0.38228	0.00833
450	0.40264	0.41915	0.50600	0.44260	0.05553
600	0.48519	0.58868	0.59018	0.55468	0.06019
900	0.69774	0.69889	0.67720	0.69128	0.01220
1200	0.71694	0.73919	0.72960	0.72858	0.01116
1800	0.68000	0.72681	0.74493	0.71725	0.03350

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

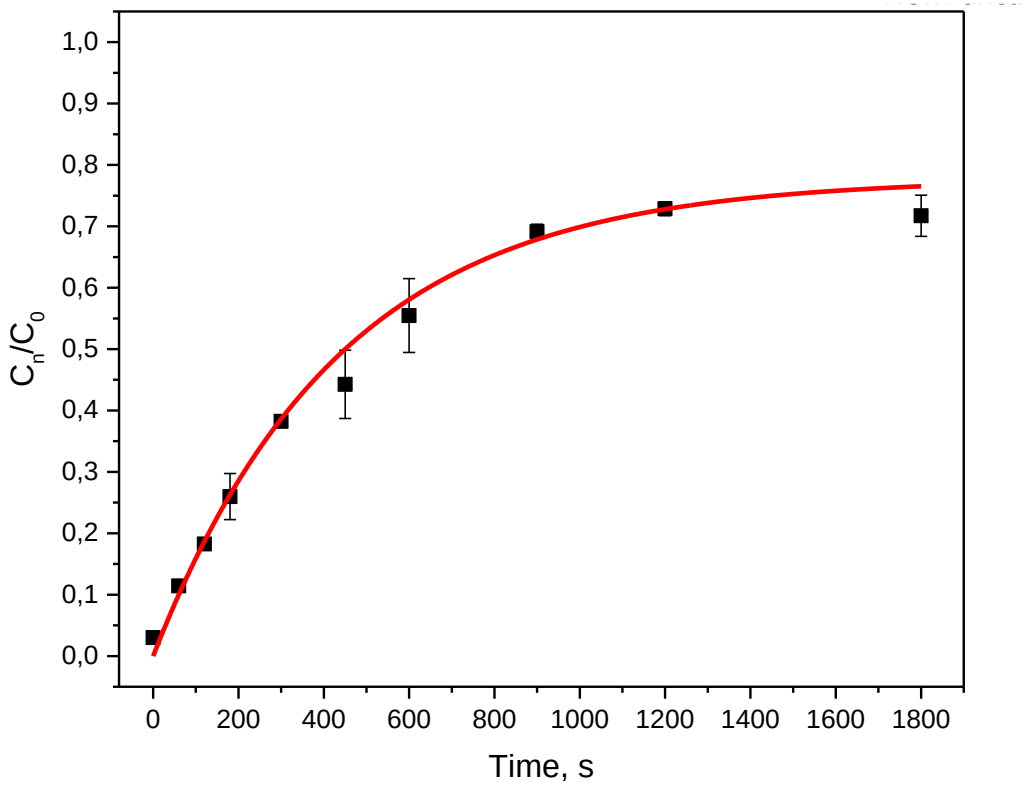


Figure S2.14. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 425 nm LED (6.02 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.97054; k_1=1.780E-3 s^{-1} (standard error 2.425E-4 s^{-1}); k_2=5.078E-4 s^{-1} (standard error 2.537E-4 s^{-1}).

Table S2.15. Data for photolysis of AlkVZ **5** using 435 nm LED (5.88 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.03637	0.03486	0.03857	0.03660	0.00187
120	0.12008	0.12302	0.13857	0.12722	0.00994
300	0.27976	0.26592	0.25486	0.26685	0.01248
600	0.43473	0.42869	0.43498	0.43280	0.00356
900	0.55310	0.54286	0.53714	0.54437	0.00809
1200	0.63102	0.61976	0.60131	0.61736	0.01500
1800	0.71384	0.69714	0.68571	0.69890	0.01415
2400	0.73641	0.70865	0.71473	0.71993	0.01459
3000	0.73878	0.73359	0.72437	0.73225	0.00730

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

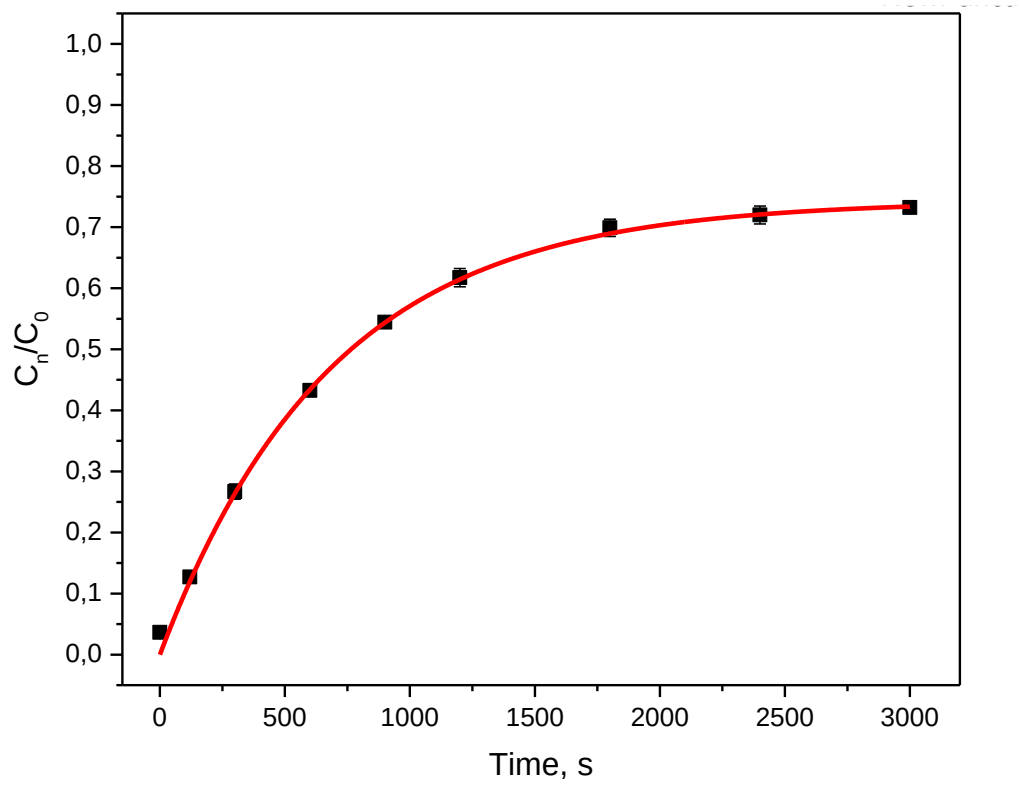


Figure S2.15. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 435 nm LED (5.88 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.98024; k_1=1.090E-3 s^{-1} (standard error 1.112E-4 s^{-1}); k_2=3.757E-4 s^{-1} (standard error 1.273E-4 s^{-1}).

Table S2.16. Data for photolysis of AlkVZ **5** using 445 nm LED (5.75 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.03633	0.03673	0.04082	0.03796	0.00248
120	0.10363	0.12653	0.10531	0.11182	0.01276
300	0.19555	0.18906	0.23441	0.20634	0.02452
600	0.37592	0.37061	0.36224	0.36959	0.00690
900	0.47306	0.46976	0.47180	0.47154	0.00167
1200	0.56061	0.54967	0.54033	0.55020	0.01015
1800	0.62902	0.63584	0.63918	0.63468	0.00518
2400	0.68992	0.68853	0.68535	0.68793	0.00234
3000	0.72151	0.70278	0.73592	0.72007	0.01662
3600	0.73261	0.74127	0.74898	0.74095	0.00819
4500	0.73343	0.74090	0.75673	0.74369	0.01190

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

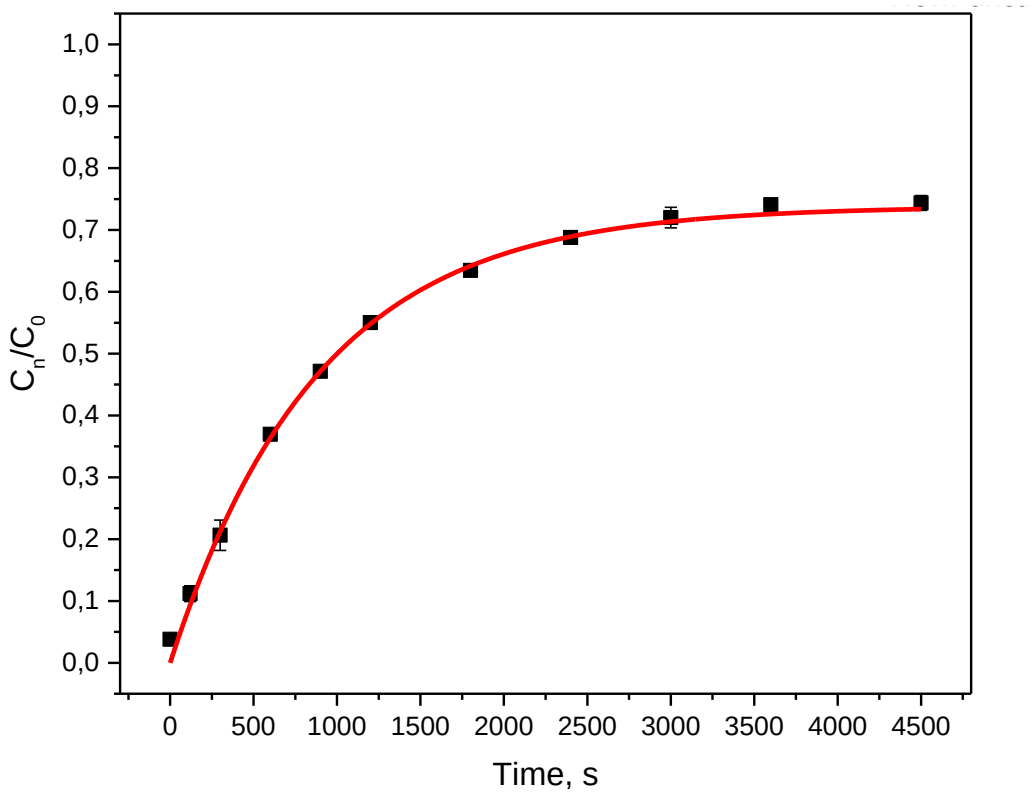


Figure S2.16. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 445 nm LED (5.75 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99364; k_1=8.343E-4 s^{-1} (standard error 3.310E-5 s^{-1}); k_2=2.957E-4 s^{-1} (standard error 3.628E-5 s^{-1}).

Table S2.17. Data for photolysis of AlkVZ **5** using 462 nm LED (5.54 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y
0	0.04041
300	0.10224
600	0.16412
1200	0.27318
1800	0.36008
2700	0.43314
3600	0.57780
4800	0.63090
6000	0.69180
7200	0.71184
8400	0.72473

Y – experimental yield of radical determined via EPR spectroscopy

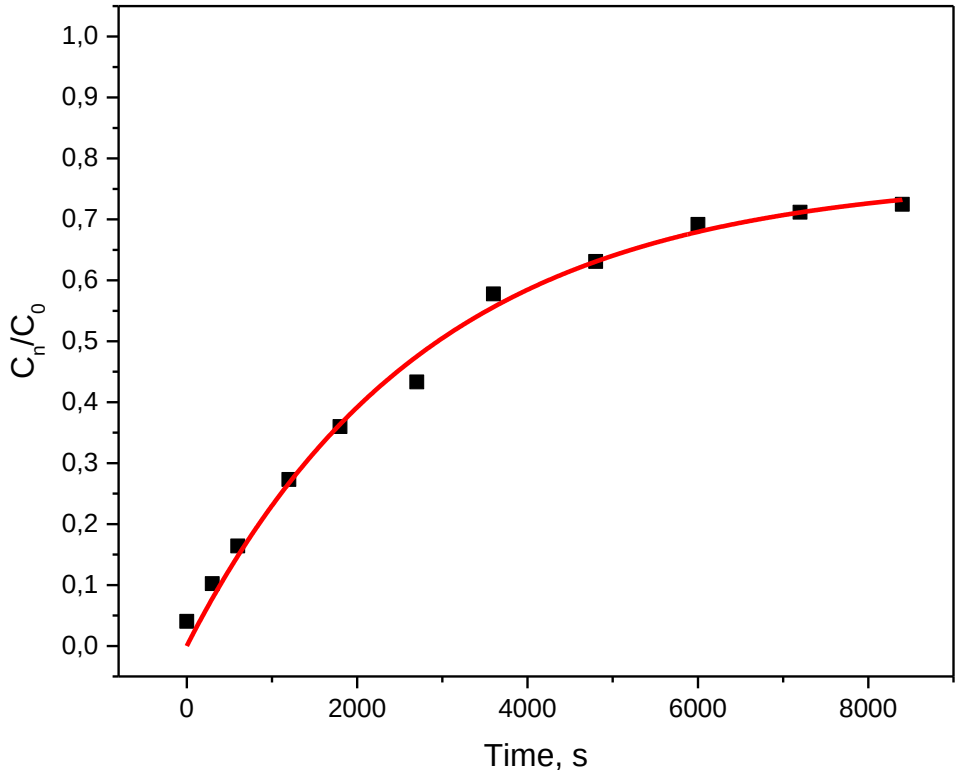


Figure S2.17. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 462 nm LED (5.54 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99155; k_1=2.734E-4 s^{-1} (standard error 1.431E-5 s^{-1}); k_2=8.091E-5 s^{-1} (standard error 1.435E-5 s^{-1}).

Table S2.18. Data for photolysis of AlkVZ **5** using 472 nm LED (5.42 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y
0	0.04417
600	0.09496
1200	0.12381
2400	0.19757
3600	0.25587
5400	0.32858
8100	0.46422
10800	0.47880
14400	0.52460

Y – experimental yield of radical determined via EPR spectroscopy

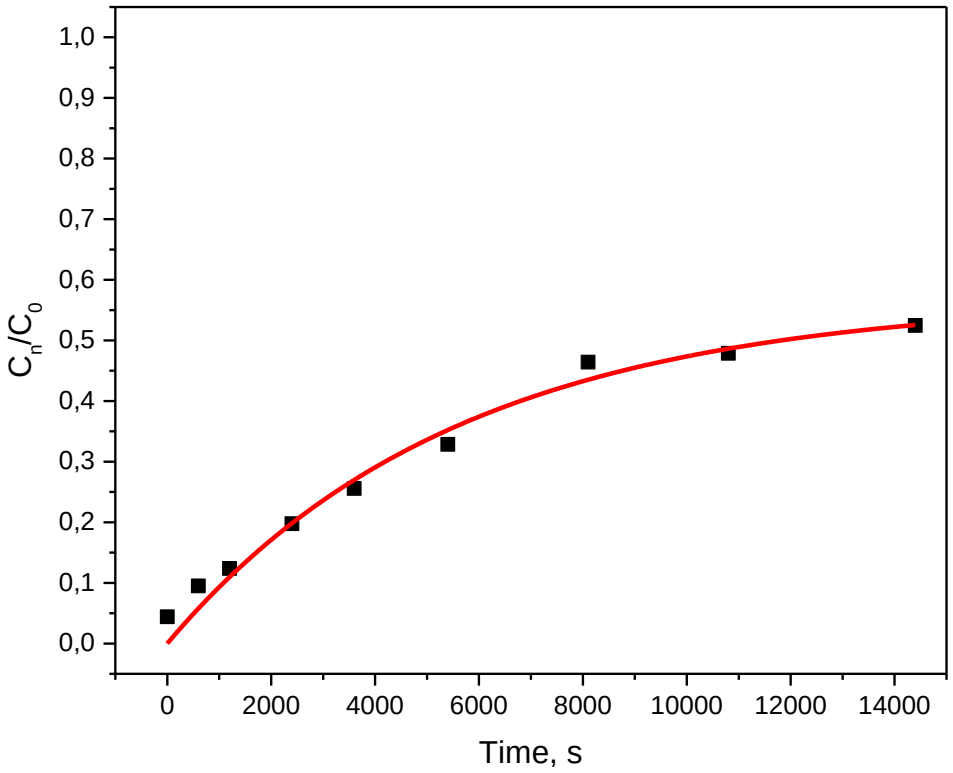


Figure S2.18. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 472 nm LED (5.42 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99155; k_1=1.017E-4 s^{-1} (standard error 9.381E-6 s^{-1}); k_2=7.705E-5 s^{-1} (standard error 1.794E-5 s^{-1}).

Table S2.19. Data for photolysis of AlkVZ **5** using 495 nm LED (5.17 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y
0	0.01325
1200	0.04651
2400	0.06696
4800	0.14134
7200	0.14664
10800	0.19108

Y – experimental yield of radical determined via EPR spectroscopy

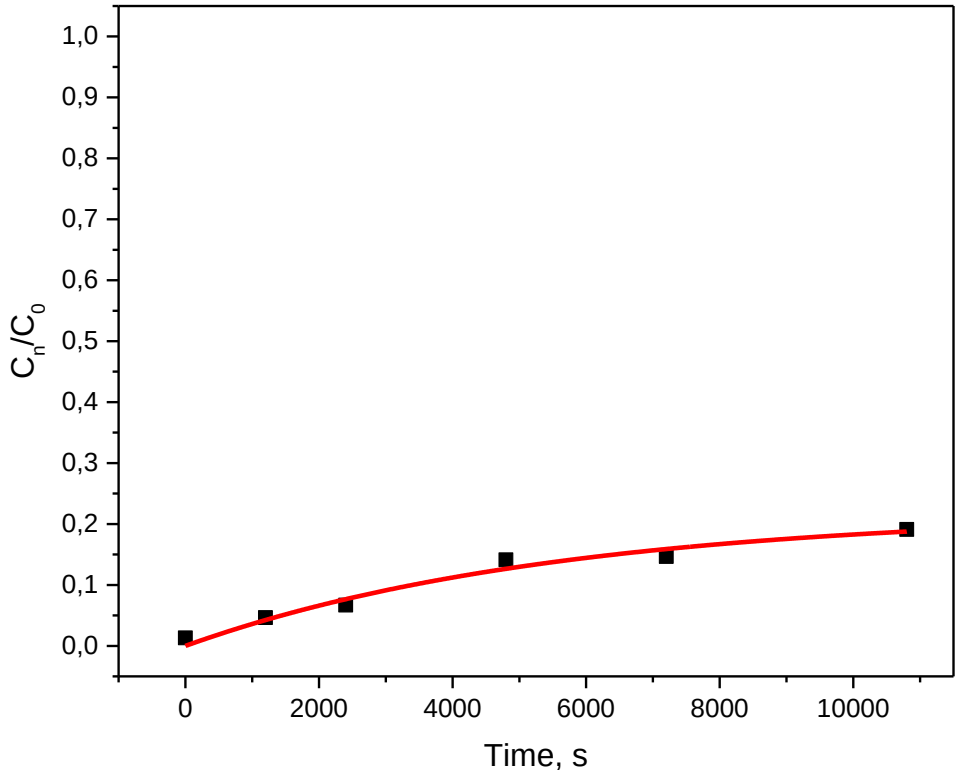


Figure S2.19. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 495 nm LED (5.17 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99155; k_1=3.928E-5 s^{-1} (standard error 6.032E-6 s^{-1}); k_2=1.398E-4 s^{-1} (standard error 4.481E-5 s^{-1}).

Table S2.20. Data for photolysis of AlkVZ **5** using 502 nm LED (5.10 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y
0	0.01315
1800	0.02901
3600	0.05326
7200	0.06591
10800	0.06618

Y – experimental yield of radical determined via EPR spectroscopy

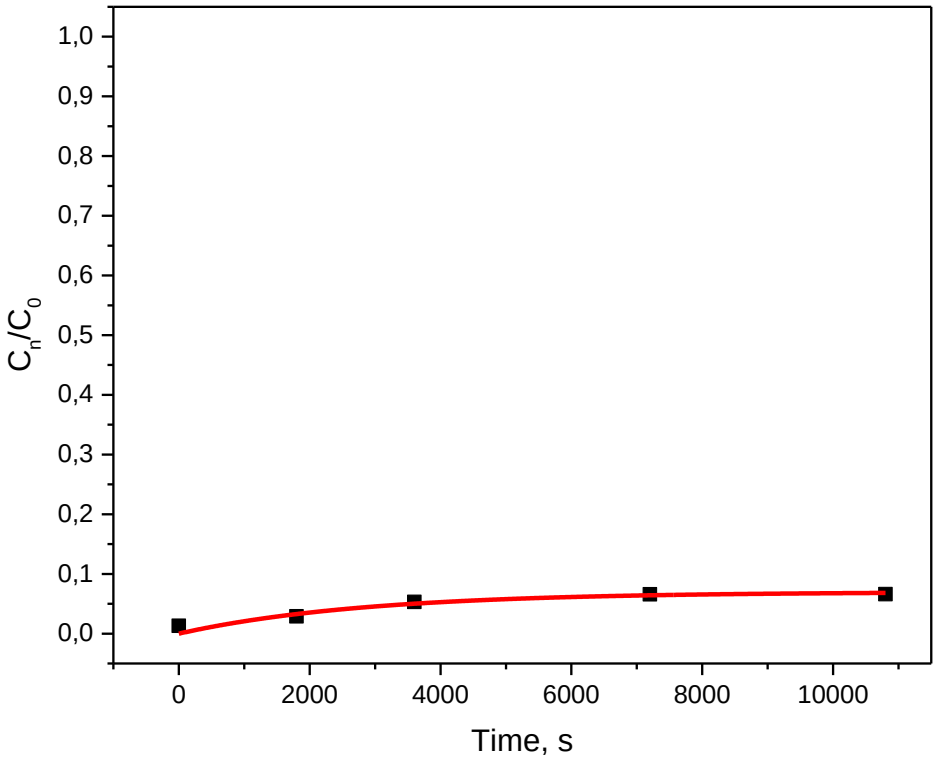


Figure S2.20. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 502 nm LED (5.10 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99155; k_1=2.459E-5 s^{-1} (standard error 6.823E-6 s^{-1}); k_2=3.279E-4 s^{-1} (standard error 1.226E-4 s^{-1}).

Table S2.21. Data for photolysis of AlkVZ **5** using 525 nm LED (4.88 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y
0	0.00272
3600	0.02112
7200	0.03105
10800	0.03345

Y – experimental yield of radical determined via EPR spectroscopy

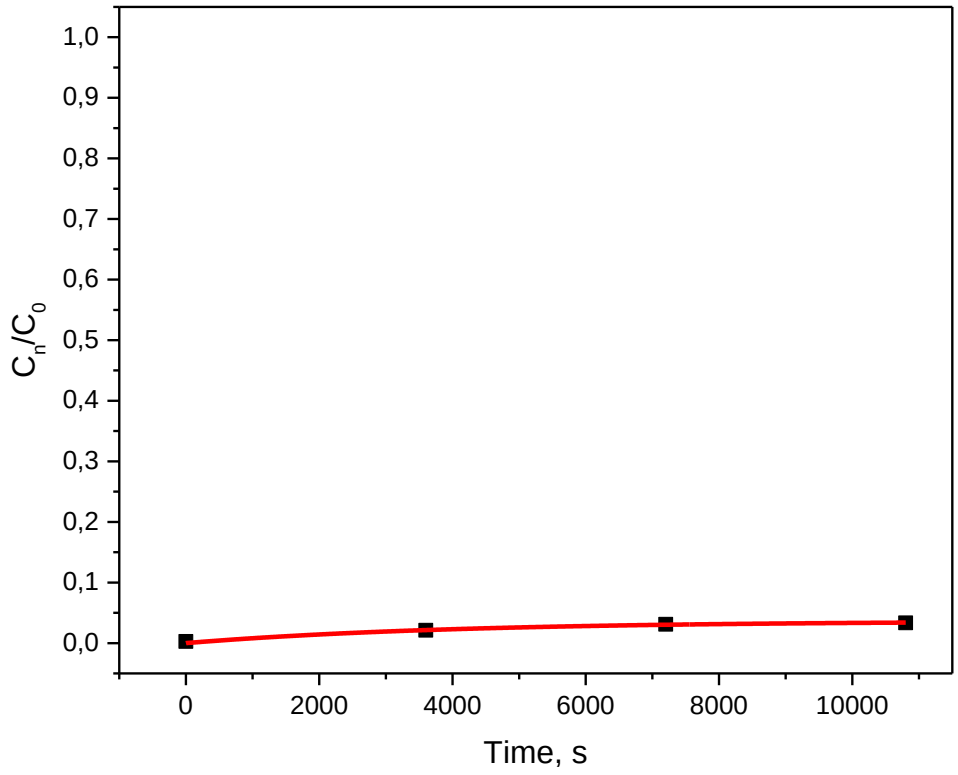


Figure S2.21. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 525 nm LED (4.88 mW power, $1.289 \cdot 10^{16}$ photons per second). R^2=0.99155; k_1=9.064E-6 s^{-1} (standard error 1.643E-6 s^{-1}); k_2=2.405E-4 s^{-1} (standard error 6.449E-5 s^{-1}).

Table S2.22. Data for photolysis of AlkVZ **5** using 560 nm LED (4.59 mW power, $1.289 \cdot 10^{16}$ photons per second).

Time, s	Y
0	0.01236
3600	0.01692
7200	0.01300
10800	0.01182

Y – experimental yield of radical determined via EPR spectroscopy

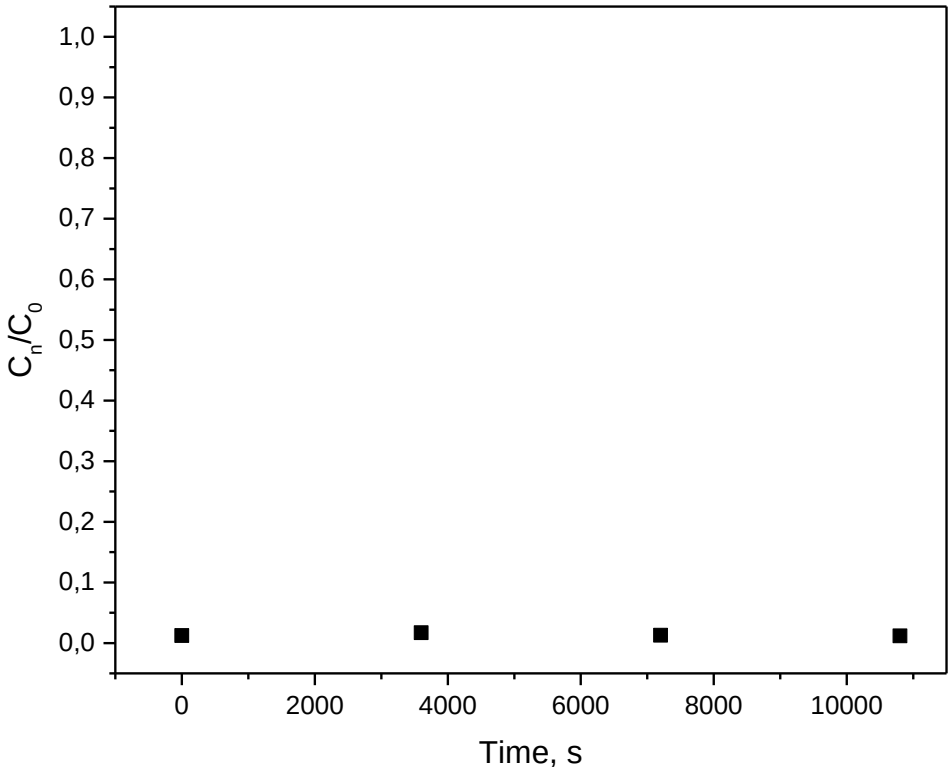


Figure S3.22. Experimental points demonstrating the absence of photolysis of AlkVZ **5** under 560 nm LED (4.59 mW power, $1.289 \cdot 10^{16}$ photons per second) irradiation. Fitting was not converged since no decomposition was observed.

Table S2.23. Data for photolysis of AlkVZ **5** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00566	0.00298	0.00500	0.00455	0.00140
30	0.04581	0.04842	0.04931	0.04785	0.00182
60	0.11230	0.10789	0.11538	0.11186	0.00376
90	0.16045	0.15551	0.16923	0.16173	0.00695
120	0.21728	0.20540	0.22554	0.21607	0.01012
180	0.29811	0.28375	0.30092	0.29426	0.00921
240	0.36906	0.34530	0.35962	0.35799	0.01196
300	0.40992	0.39354	0.41769	0.40705	0.01233
450	0.48879	0.48635	0.47908	0.48474	0.00505
600	0.52660	0.52614	0.50685	0.51986	0.01127
900	0.55264	0.54579	0.55338	0.55060	0.00418
1200	0.56279	0.55288	0.54365	0.55311	0.00957
1800	0.53925	0.56579	0.51688	0.54064	0.02448
2400	0.52075	0.54330	0.51908	0.52771	0.01353
3000	0.50385	0.53888	0.50000	0.51424	0.02142

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

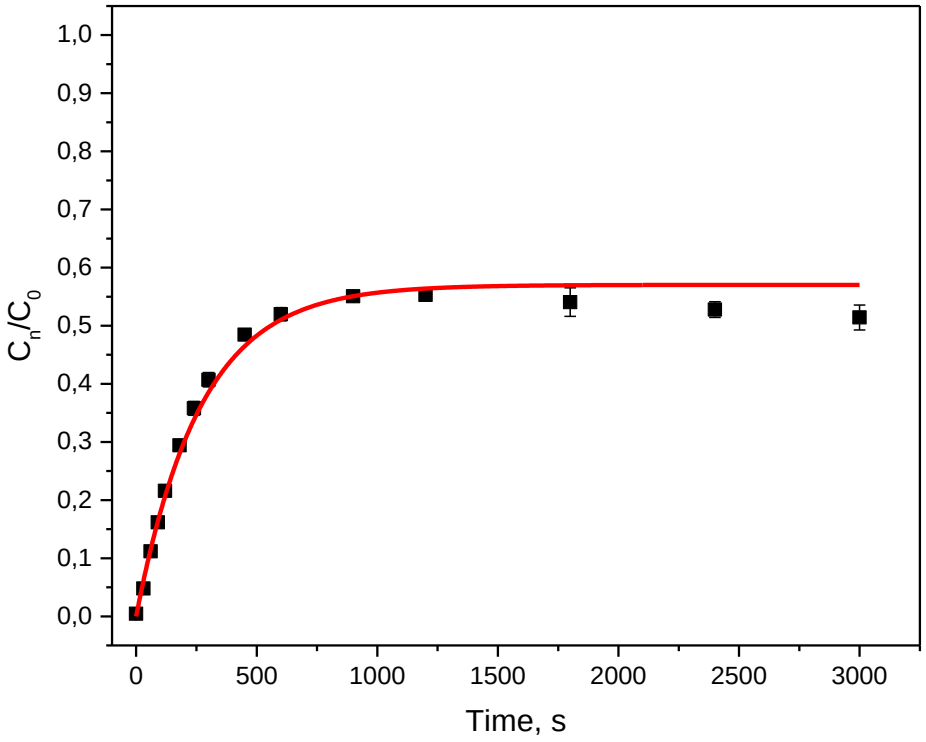


Figure S2.23. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.99619; k_1=2.140E-3 s^{-1} (standard error 9.773E-5 s^{-1}); k_2=1.610E-3 s^{-1} (standard error 1.305E-4 s^{-1}).

Table S2.24. Data for photolysis of AlkVZ **5** using 365 nm LED (420 μW power, $7.753 \cdot 10^{14}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00985	0.01294	0.01176	0.01152	0.00156
60	0.03451	0.03697	0.03606	0.03585	0.00124
120	0.05672	0.06121	0.06162	0.05985	0.00272
300	0.12400	0.11903	0.12588	0.12297	0.00354
600	0.21582	0.20129	0.21441	0.21051	0.00801
900	0.28358	0.27147	0.27471	0.27659	0.00627
1200	0.33612	0.31256	0.33647	0.32838	0.01370
1800	0.40543	0.39756	0.41576	0.40625	0.00913
2700	0.45833	0.46529	0.46356	0.46239	0.00362
3600	0.44776	0.47741	0.47946	0.46821	0.01774
4800	0.48701	0.48341	0.49753	0.48932	0.00734
6000	0.48934	0.49932	0.49964	0.49610	0.00586

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

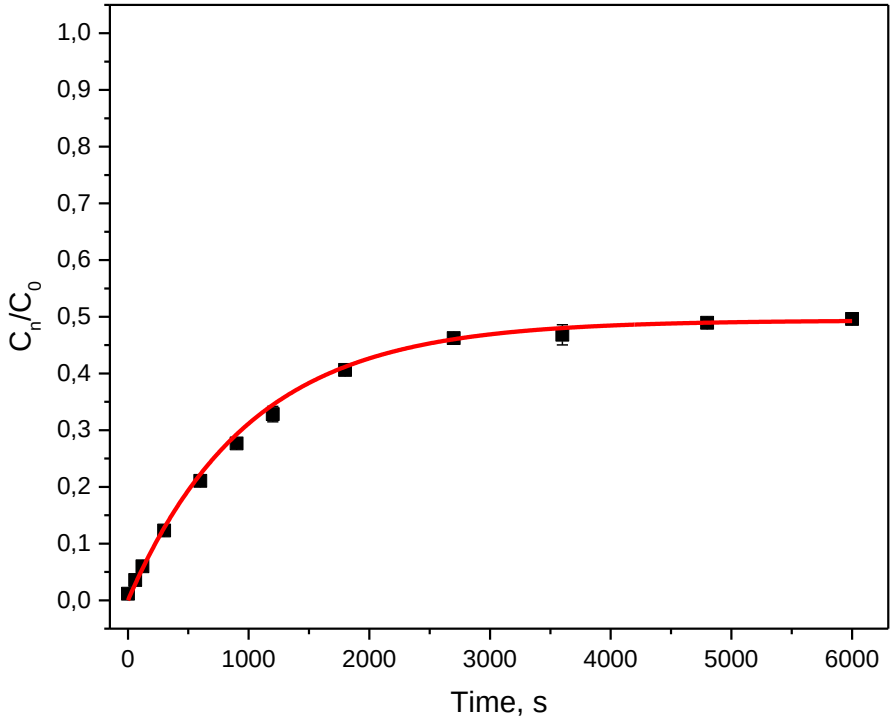


Figure S2.24. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 365 nm LED (420 μW power, $7.753 \cdot 10^{14}$ photons per second). R^2=0.99562; k_1=4.927E-4 s^{-1} (standard error 2.753E-5 s^{-1}); k_2=5.053E-4 s^{-1} (standard error 4.400E-5 s^{-1}).

Table S2.25. Data for photolysis of AlkVZ **5** using 405 nm LED (380 μW power, $7.753 \cdot 10^{14}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00856	0.01690	0.01065	0.01204	0.00434
60	0.01249	0.02020	0.01479	0.01583	0.00396
300	0.03202	0.04085	0.03769	0.03685	0.00447
600	0.05913	0.06896	0.06608	0.06472	0.00505
1200	0.11273	0.11763	0.12493	0.11843	0.00614
2400	0.20474	0.20845	0.21915	0.21078	0.00748
3600	0.27198	0.26761	0.27048	0.27002	0.00222
5400	0.31877	0.30879	0.31173	0.31310	0.00513
6600	0.34064	0.32394	0.32358	0.32939	0.00975
7800	0.35051	0.35118	0.34823	0.34997	0.00155
9600	0.36991	0.36580	0.36175	0.36582	0.00408
11400	0.38754	0.37465	0.37361	0.37860	0.00776
13200	0.39880	0.38270	0.38358	0.38836	0.00905
15000	0.40770	0.39479	0.38989	0.39746	0.00920
16800	0.40809	0.40845	0.40434	0.40696	0.00228
18600	0.39770	0.38225	0.40324	0.39440	0.01088

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

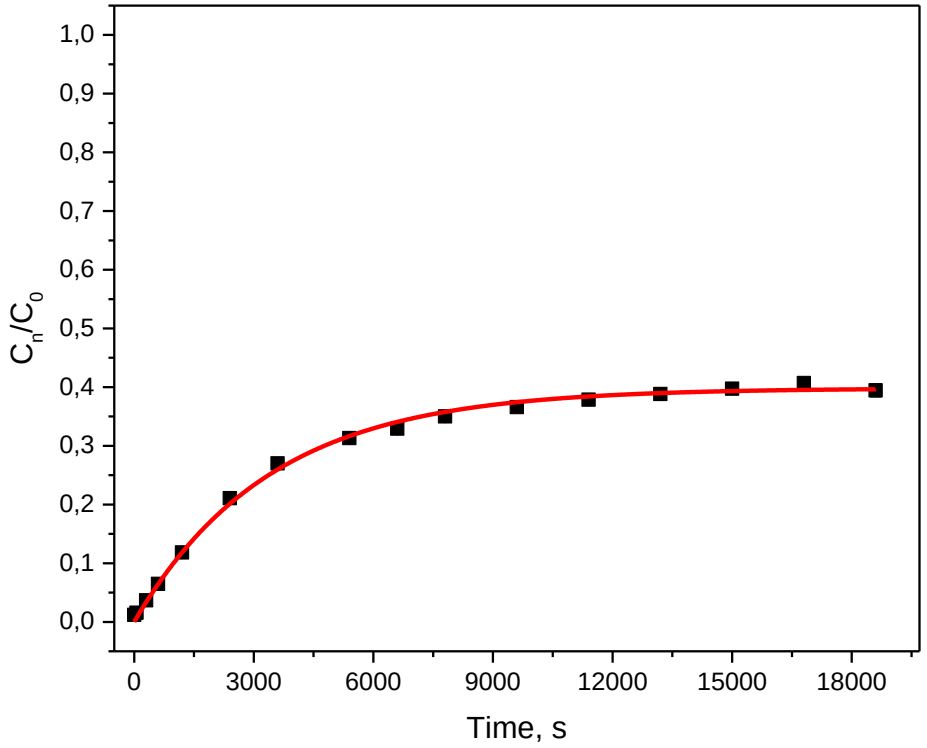


Figure S2.25. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **5** using 405 nm LED (380 μW power, $7.753 \cdot 10^{14}$ photons per second). R^2=0.99491; k_1=1.169E-4 s^{-1} (standard error 4,105E-6 s^{-1}); k_2= 1.766E-4 s^{-1} (standard error 9.139E-6 s^{-1}).

AlkVZ 2

Table S2.26. Data for photolysis of AlkVZ **2** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00556	0.00575	0.00543	0.00558	0.000161
5	0.22495	0.23547	0.21925	0.226557	0.008228
10	0.37245	0.38097	0.35999	0.371137	0.010551
20	0.52705	0.51852	0.51185	0.51914	0.007619
30	0.60346	0.60109	0.59045	0.598333	0.006929
45	0.65998	0.65016	0.64454	0.65156	0.007815
60	0.65645	0.67573	0.67353	0.66857	0.010554
90	0.66245	0.67976	0.6764	0.67287	0.009179

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

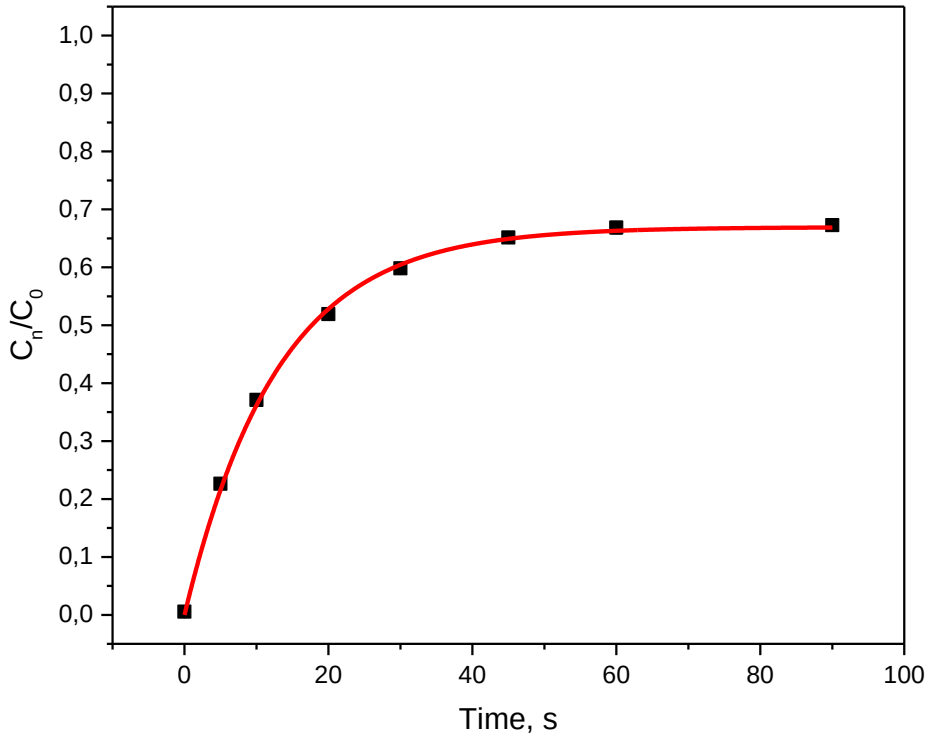


Figure S2.26. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **2** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99845; k_1=5.207E-2 s^{-1} (standard error 3.160E-3 s^{-1}); k_2=2.573E-2 s^{-1} (standard error 2.790E-3 s^{-1}).

Table S2.27. Data for photolysis of AlkVZ **2** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00613	0.00636	0.00615	0.00621	0.00013
30	0.11503	0.12424	0.11059	0.11662	0.00696
60	0.18558	0.19939	0.19928	0.19475	0.00794
120	0.29448	0.29697	0.31002	0.30049	0.00835
180	0.37546	0.38788	0.37041	0.37792	0.00899
300	0.50000	0.50273	0.48800	0.49691	0.00784
450	0.57218	0.57333	0.57248	0.57266	0.00060
600	0.60939	0.59606	0.59880	0.60142	0.00704
900	0.62485	0.60767	0.63607	0.62286	0.01430
1200	0.64693	0.63691	0.62236	0.63540	0.01235
1800	0.63497	0.64409	0.63971	0.63959	0.00456
2400	0.64141	0.64985	0.64676	0.64601	0.00427

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

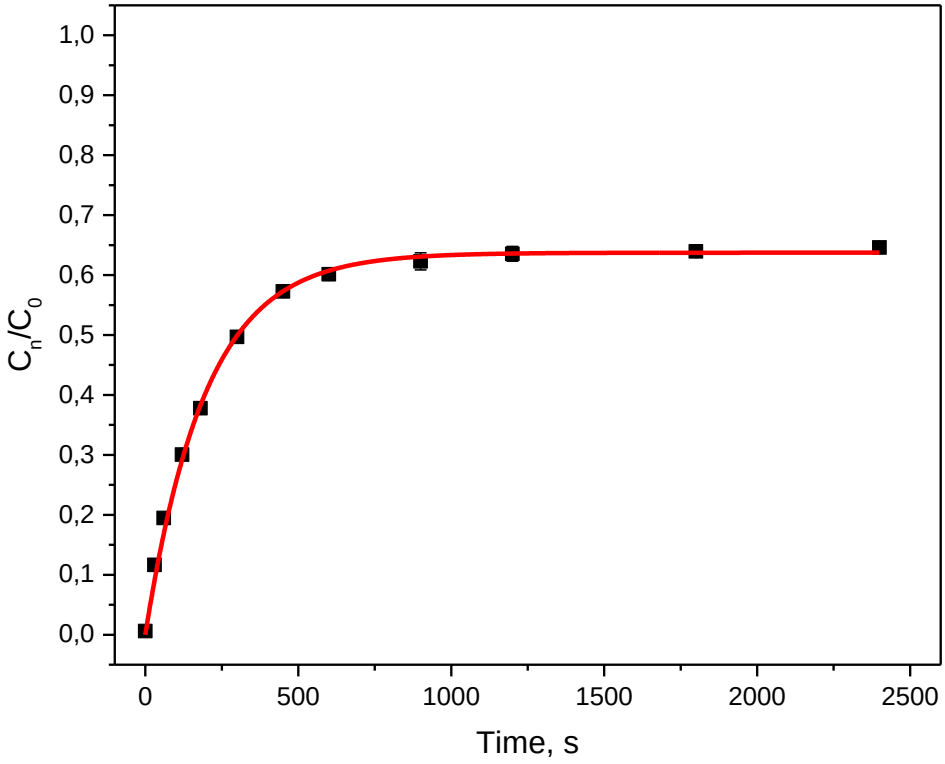


Figure S2.27. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **2** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.99968; k_1=3.250E-3 s^{-1} (standard error 1.063E-4 s^{-1}); k_2=1.850E-3 s^{-1} (standard error 1.150E-4 s^{-1}).

AlkVZ 3

Table S2.28. Data for photolysis of AlkVZ **3** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.23055	0.22773	0.19116	0.21648	0.02197
5	0.40294	0.38739	0.37884	0.38972	0.01222
10	0.58824	0.56239	0.56071	0.57045	0.01543
20	0.70315	0.68697	0.70768	0.69927	0.01089
30	0.73865	0.73235	0.74826	0.73975	0.00801
45	0.75294	0.73971	0.78361	0.75875	0.02252
60	0.75630	0.75210	0.76763	0.75868	0.00803
90	0.73782	0.75601	0.76826	0.75403	0.01532

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

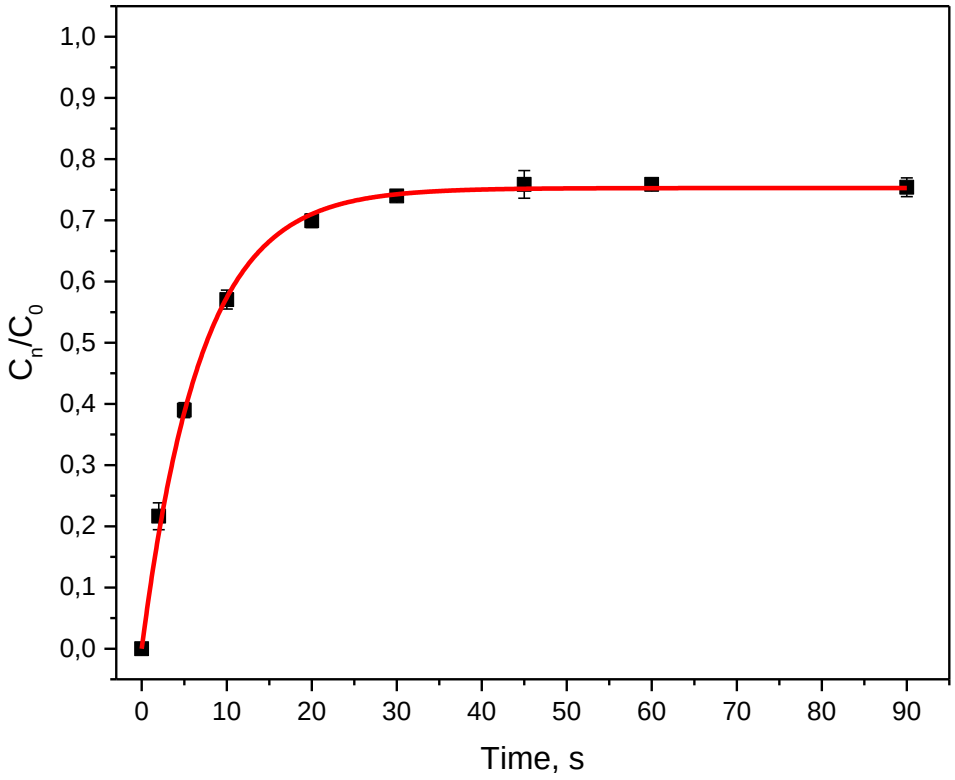


Figure S2.28. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **3** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99984; k_1=1.082E-1 s^{-1} (standard error 2.710E-3 s^{-1}); k_2=3.552E-2 s^{-1} (standard error 1.330E-3 s^{-1}).

Table S2.29. Data for photolysis of AlkVZ **3** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00837	0.01097	0.01092	0.01009	0.00149
10	0.08868	0.09367	0.08952	0.09062	0.00267
30	0.21109	0.22278	0.21031	0.21473	0.00699
60	0.33180	0.35443	0.33624	0.34082	0.01199
90	0.44372	0.44962	0.44410	0.44581	0.00330
120	0.49958	0.53143	0.50579	0.51227	0.01688
180	0.61715	0.60970	0.62009	0.61565	0.00536
240	0.65544	0.66608	0.64279	0.65477	0.01166
300	0.69916	0.69451	0.67555	0.68974	0.01251
450	0.73640	0.72532	0.69869	0.72014	0.01938
600	0.74561	0.72785	0.71616	0.72987	0.01483
900	0.72803	0.74008	0.73624	0.73478	0.00616

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

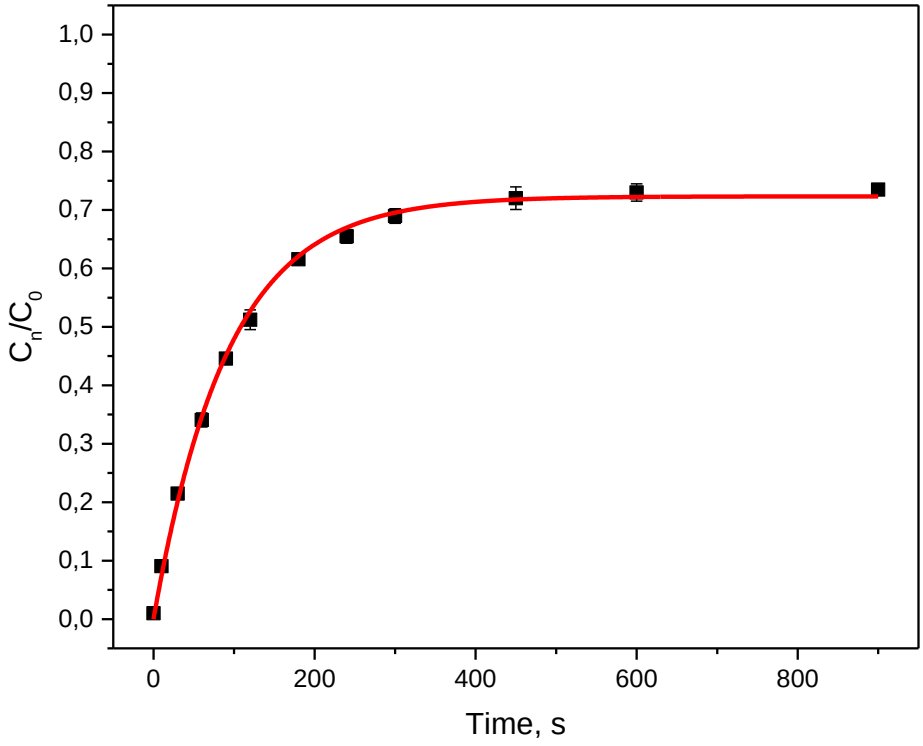


Figure S2.29. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **3** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.9974; k_1=7.860E-3 s^{-1} (standard error 2.834E-4 s^{-1}); k_2=3.010E-3 s^{-1} (standard error 2.911E-4 s^{-1}).

AlkVZ 4

Table S2.30. Data for photolysis of AlkVZ **4** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.01247	0.01271	0.01410	0.01309	0.00088
5	0.11613	0.11441	0.12016	0.11690	0.00295
10	0.20925	0.20890	0.22117	0.21311	0.00699
15	0.28903	0.29703	0.30261	0.29622	0.00683
20	0.35140	0.34534	0.36953	0.35542	0.01259
30	0.41914	0.42203	0.42992	0.42370	0.00558
45	0.46624	0.45890	0.47643	0.46719	0.00880
60	0.47699	0.46928	0.49242	0.47956	0.01178
90	0.50323	0.49250	0.47980	0.49184	0.01173
120	0.49376	0.50000	0.48085	0.49154	0.00977
180	0.49462	0.50487	0.47391	0.49113	0.01577

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

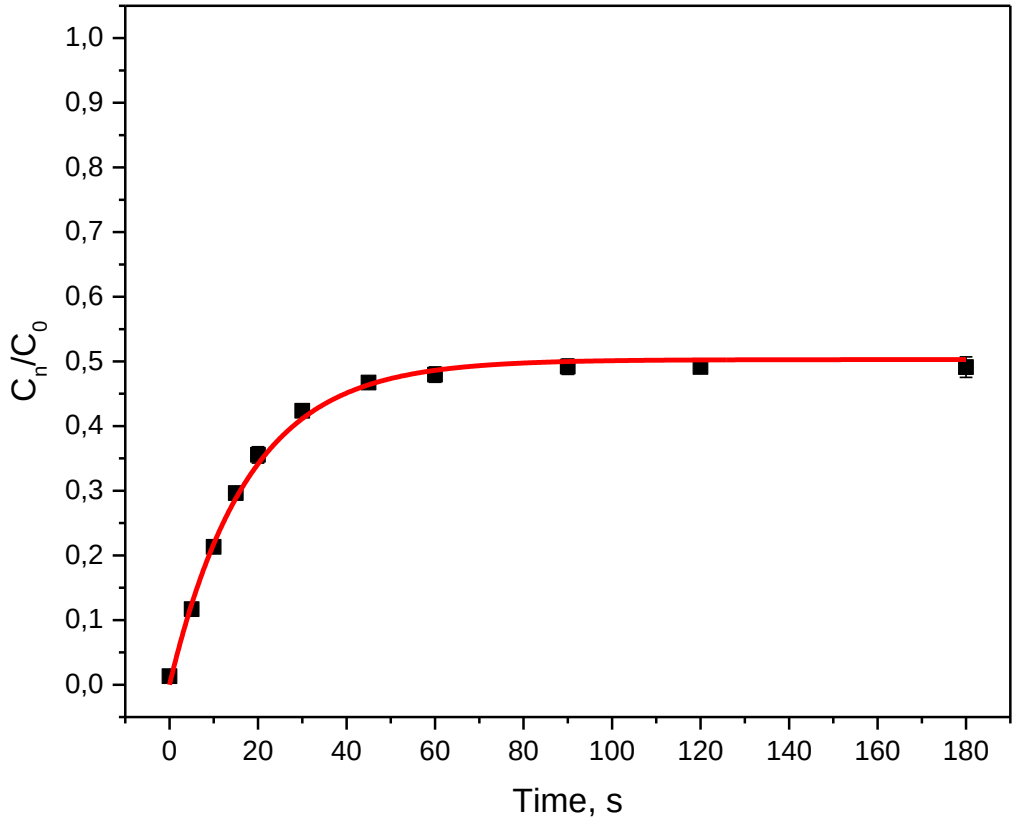


Figure S2.30. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **4** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99466; k_1=2.858E-2 s^{-1} (standard error 1.370E-3 s^{-1}); k_2=2.825E-2 s^{-1} (standard error 2.520E-3 s^{-1}).

Table S2.31. Data for photolysis of AlkVZ **4** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.01095	0.01304	0.01410	0.01270	0.00160
30	0.06862	0.07304	0.06784	0.06983	0.00280
60	0.11955	0.11826	0.11366	0.11716	0.00310
120	0.21722	0.21304	0.19824	0.20950	0.00997
180	0.28205	0.28348	0.27577	0.28043	0.00410
300	0.38266	0.37957	0.38458	0.38227	0.00253
450	0.43991	0.45565	0.43537	0.44364	0.01064
600	0.47043	0.48826	0.46916	0.47595	0.01068
900	0.50474	0.50174	0.50176	0.50275	0.00173
1200	0.53168	0.53587	0.53458	0.53404	0.00215
1800	0.53357	0.53287	0.54537	0.53727	0.00702
2400	0.52200	0.53726	0.52863	0.52930	0.00765

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

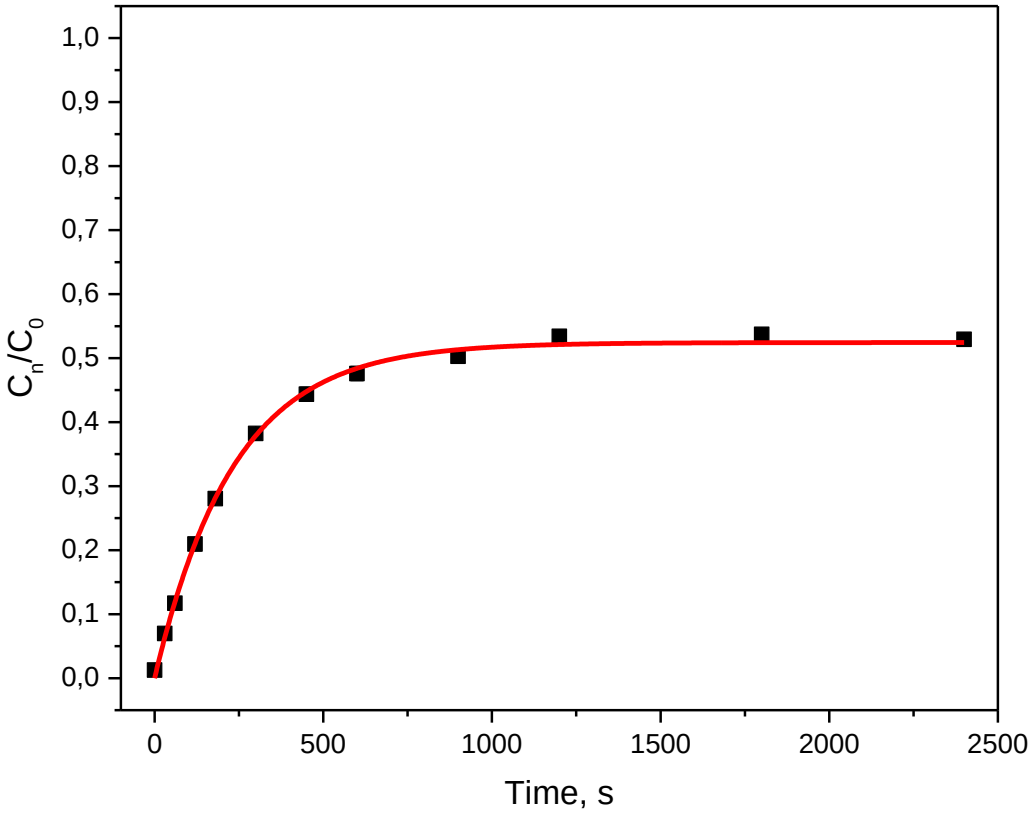


Figure S2.31. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **4** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.99773; k_1=2.240E-3 s^{-1} (standard error 9,316E-5 s^{-1}); k_2=2.030E-3 s^{-1} (standard error 1.123E-4 s^{-1}).

AlkVZ 6

Table S2.32. Data for photolysis of AlkVZ **6** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00515	0.00405	0.00281	0.00400	0.00117
5	0.15152	0.17396	0.18078	0.16875	0.01531
10	0.26576	0.33974	0.31247	0.30599	0.03741
20	0.45152	0.47028	0.47162	0.46447	0.01124
30	0.58379	0.58729	0.58392	0.58500	0.00198
45	0.66212	0.68105	0.64520	0.66279	0.01793
60	0.71930	0.73067	0.70255	0.71751	0.01415
90	0.74788	0.74588	0.72718	0.74031	0.01142
120	0.73536	0.72094	0.72686	0.72772	0.00725
180	0.70355	0.71689	0.71751	0.71265	0.00789

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

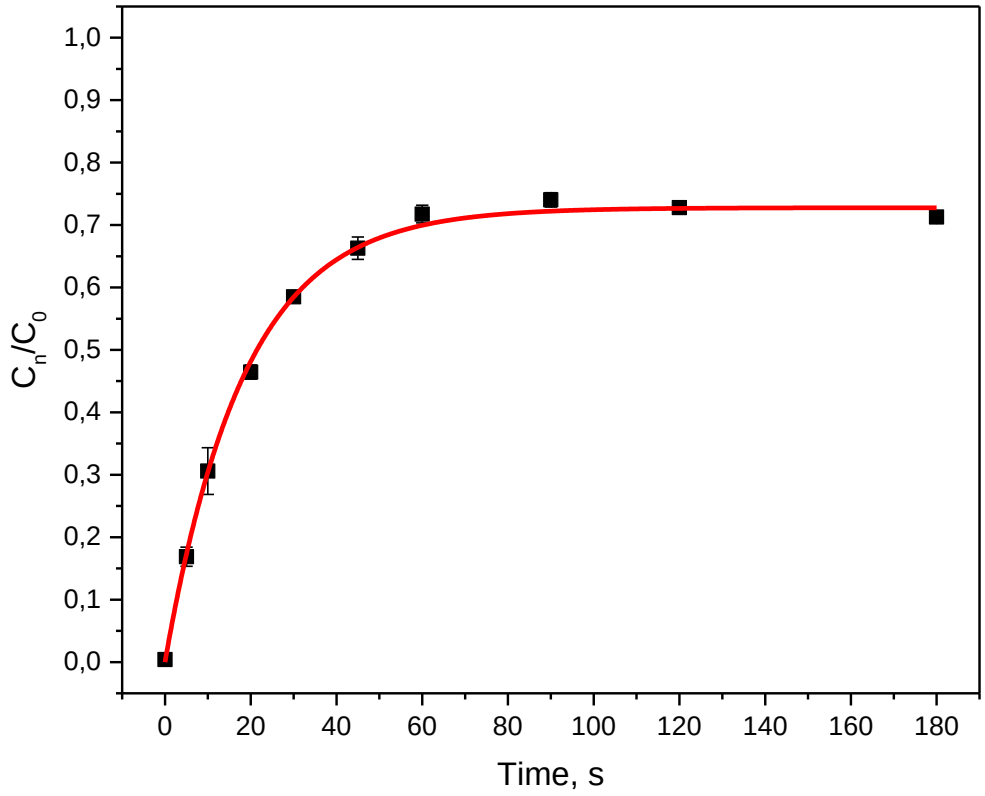


Figure S2.32. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **6** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99969; k_1=3.944E-2 s^{-1} (standard error 8.462E-4 s^{-1}); k_2=1.476E-2 s^{-1} (standard error 8,567E-4 s^{-1}).

Table S2.33. Data for photolysis of AlkVZ **6** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00556	0.00499	0.00572	0.00542	0.00038
30	0.07645	0.08120	0.07946	0.07904	0.00240
60	0.14376	0.13973	0.13466	0.13938	0.00456
120	0.24400	0.24105	0.23964	0.24156	0.00222
180	0.32180	0.32481	0.32622	0.32428	0.00226
300	0.43218	0.43068	0.43544	0.43277	0.00243
450	0.53985	0.52890	0.54378	0.53751	0.00771
600	0.57684	0.59850	0.60451	0.59328	0.01455
900	0.67164	0.66000	0.67733	0.66966	0.00883
1200	0.65865	0.70647	0.70118	0.68877	0.02622
1800	0.70905	0.68827	0.68776	0.69503	0.01215
2400	0.67729	0.67579	0.71747	0.69018	0.02364

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

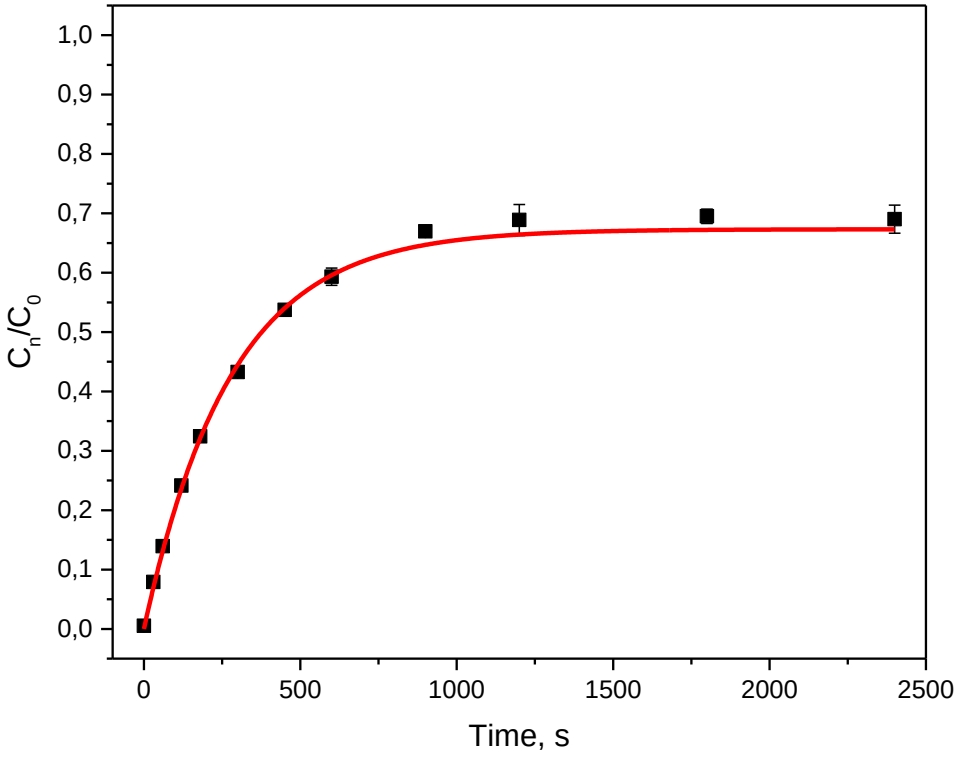


Figure S2.33. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **6** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.99802; k_1=2.430E-3 s^{-1} (standard error 5.825E-5 s^{-1}); k_2=1.180E-3 s^{-1} (standard error 1.274E-4 s^{-1}).

AlkVZ 7

Table S2.34. Data for photolysis of AlkVZ **7** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00669	0.00783	0.00781	0.00744	0.00065
5	0.19703	0.15967	0.18516	0.18062	0.01909
10	0.31524	0.30252	0.30703	0.30826	0.00645
20	0.42454	0.41093	0.41445	0.41664	0.00706
30	0.50446	0.48294	0.50645	0.49795	0.01304
45	0.58327	0.57451	0.55430	0.57069	0.01486
60	0.60967	0.61972	0.59648	0.60862	0.01166
90	0.59851	0.63674	0.62344	0.61956	0.01941
120	0.63729	0.64457	0.61414	0.63200	0.01589
180	0.59963	0.65005	0.59375	0.61448	0.03095

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

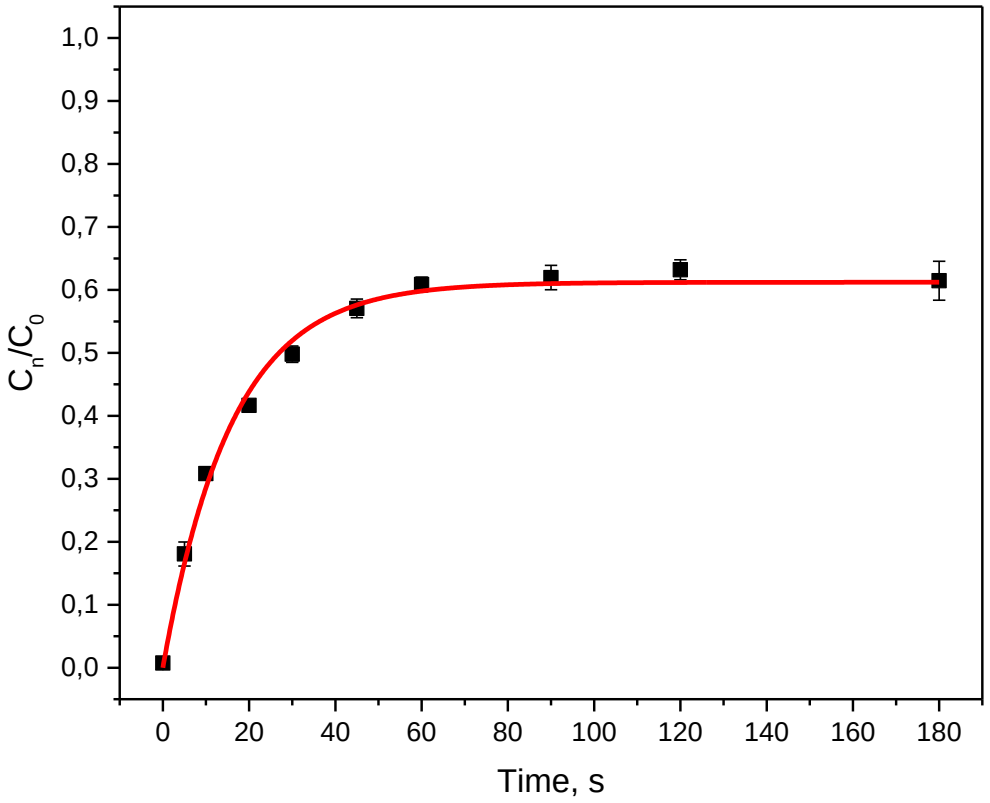


Figure S2.34. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **7** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99292; k_1=3.855E-2 s^{-1} (standard error 3.040E-3 s^{-1}); k_2=2.443E-2 s^{-1} (standard error 4,030E-3 s^{-1}).

Table S2.35. Data for photolysis of AlkVZ **7** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.01062	0.00607	0.00435	0.00701	0.00324
30	0.09207	0.08214	0.08261	0.08561	0.00560
60	0.14873	0.14286	0.15725	0.14961	0.00724
120	0.25708	0.25357	0.26087	0.25717	0.00365
180	0.31622	0.32357	0.33116	0.32365	0.00747
300	0.40262	0.42196	0.42391	0.41616	0.01177
450	0.48336	0.49036	0.49094	0.48822	0.00422
600	0.53152	0.53857	0.54130	0.53713	0.00505
900	0.59490	0.59250	0.58333	0.59024	0.00611
1200	0.61172	0.61536	0.60942	0.61217	0.00300
1800	0.60552	0.61643	0.60761	0.60985	0.00579
2400	0.64235	0.64536	0.61594	0.63455	0.01619
3000	0.61792	0.62179	0.61232	0.61734	0.00476

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

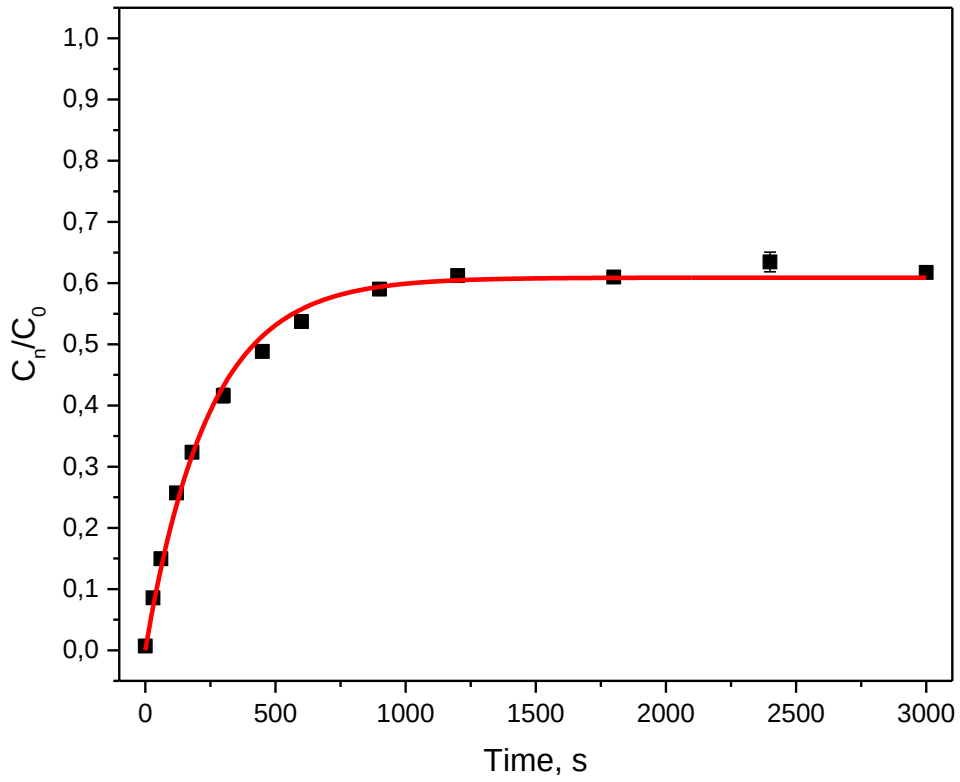


Figure S2.35. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **7** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.99607; k_1=2.510E-3 s^{-1} (standard error 1.067E-4 s^{-1}); k_2=1.610E-3 s^{-1} (standard error 9.737E-5 s^{-1}).

AlkVZ 8

Table S2.36. Data for photolysis of AlkVZ **8** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00502	0.00873	0.00953	0.00776	0.00241
5	0.14431	0.15642	0.15041	0.15038	0.00606
10	0.26497	0.26594	0.27804	0.26965	0.00728
15	0.33892	0.34061	0.34846	0.34266	0.00509
20	0.39854	0.39786	0.40372	0.40004	0.00321
30	0.47136	0.48035	0.47887	0.47686	0.00482
45	0.51965	0.53218	0.53227	0.52803	0.00726
60	0.55949	0.55079	0.56050	0.55693	0.00534
90	0.56564	0.56070	0.55977	0.56204	0.00316
120	0.57504	0.54397	0.56540	0.56147	0.01590
180	0.54569	0.53913	0.54742	0.54408	0.00437
240	0.54640	0.53275	0.53486	0.53800	0.00735

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

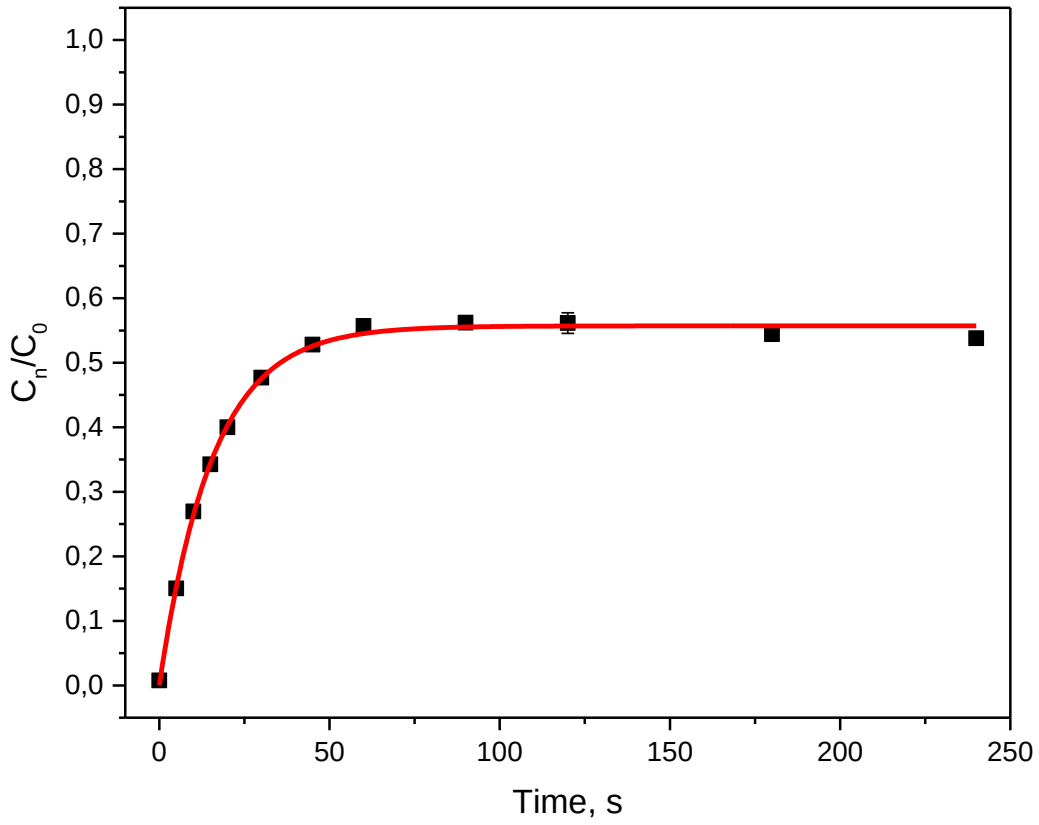


Figure S2.36. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **8** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.99871; k_1=3.567E-2 s^{-1} (standard error 8.452E-4 s^{-1}); k_2=2.836E-2 s^{-1} (standard error 9,781E-4 s^{-1}).

Table S2.37. Data for photolysis of AlkVZ **8** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second).

Time, s	Y_1	Y_2	Y_3	Y_{av}	Y_{sd}
0	0.00819	0.00793	0.01068	0.00893	0.00152
30	0.04853	0.05163	0.06370	0.05462	0.00801
60	0.10181	0.10890	0.11516	0.10862	0.00668
120	0.19306	0.19057	0.19484	0.19282	0.00214
300	0.29622	0.26762	0.28658	0.28347	0.01455
450	0.31492	0.30515	0.30091	0.30699	0.00718
600	0.32462	0.31278	0.32028	0.31923	0.00599
900	0.32773	0.32159	0.30982	0.31971	0.00910
1200	0.30412	0.28868	0.29455	0.29578	0.00779
1800	0.27403	0.26969	0.26993	0.27122	0.00244

Y_1, Y_2, Y_3 – experimental yield of radical determined via EPR spectroscopy; Y_{av} – average yield of radical; Y_{sd} – standard deviation of the experimental yield of radical.

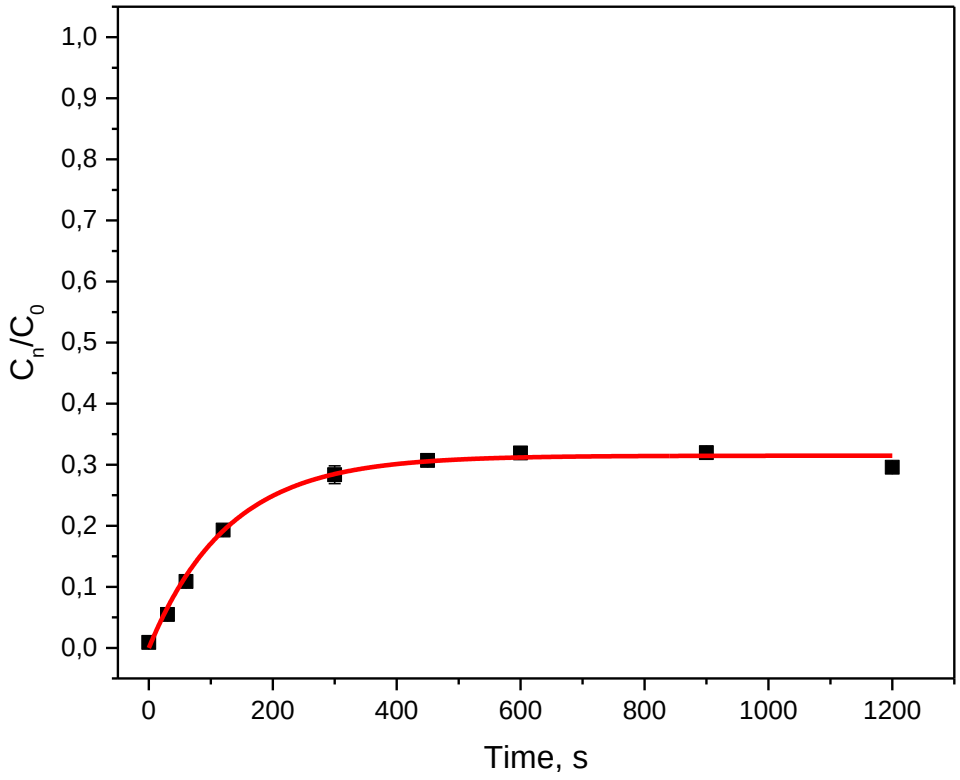


Figure S2.37. Experimental points and fitted curve for competitive first order homolysis reactions of AlkVZ **8** using 405 nm LED (5.42 mW power, $1.105 \cdot 10^{16}$ photons per second). R^2=0.9941; k_1=2.460E-3 s^{-1} (standard error 1.266E-4 s^{-1}); k_2=5.370E-3 s^{-1} (standard error 4.501E-5 s^{-1}).

Table S2.38. Integral quantum yields Φ of homolysis reactions of AlkVZ **1** and AlkVZ **5** under LED irradiation with power of $1.562 \cdot 10^{17}$ photons per second, calculated for 95 % conversion of the initial AlkVZ.

λ, nm	Φ, %	
	AlkVZ **1**	AlkVZ **5**
365	2.280	0.561
405	2.600	0.376
455	8.960	0.318
530	0.000	0.003

Table S2.39. Integral quantum yields Φ of homolysis reactions of AlkVZ **5** under LED irradiation with power of $1.289 \cdot 10^{16}$ photons per second, calculated for 95 % conversion of the initial AlkVZ.

λ, nm	Φ, %
367	0.678
382	0.573
392	0.511
405	0.390
415	0.319
425	0.219
435	0.161
445	0.171
462	0.138
472	0.099
495	0.118
502	0.086
525	0.038
560	0.000

Section S3. Kinetics of Verdazyl Radical Decay under Light Irradiation

1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical 15

Table S3.1. Decomposition of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	C, M [a]
0	6.275E-04
60	6.330E-04
300	6.286E-04
600	6.159E-04
900	6.014E-04
1200	5.887E-04
1500	5.670E-04
1800	5.534E-04
2400	5.160E-04
3000	4.649E-04
3600	3.853E-04
4800	1.723E-04

[a] *Molar concentration of radical.*

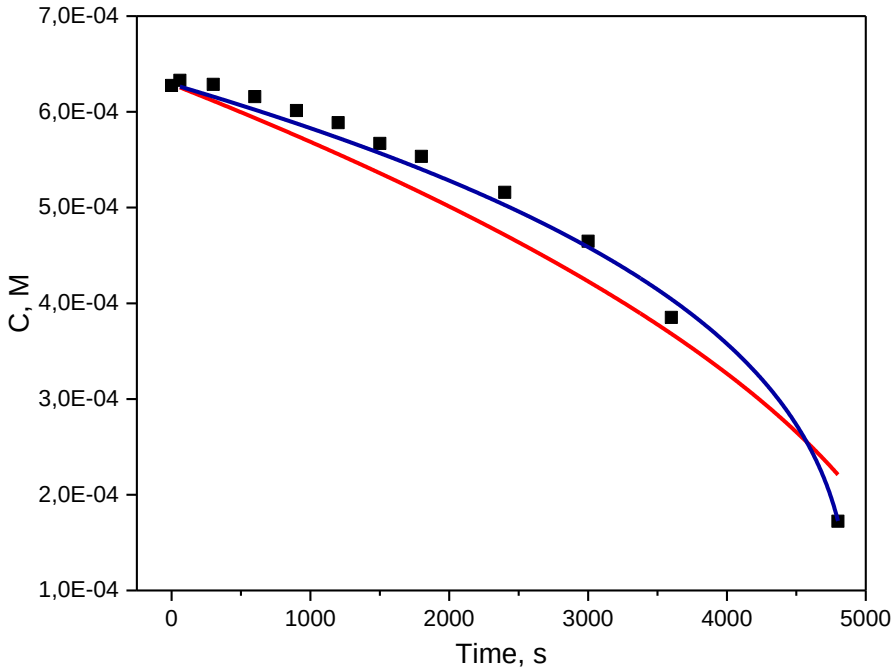


Figure S3.1. Experimental points and fitted curves for negative first order (red) decomposition reaction of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** (R^2=0.93994; k_3=3.613E-11 s^{-1}; standard error 1.296E-6 s^{-1}) and negative second order (blue) decomposition reaction (R^2=0.99115; k_3=1.692E-14 s^{-1}; standard error 7.287E-17 s^{-1}) using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second).

Table S3.2. Decomposition of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** using 405 nm LED (76 mW power, 1.562·1017 photons per second).

Time, s	C_n/C_0[a]
0	1.00000
60	1.00396
120	1.00508
300	0.99993
600	0.99604
900	0.98724
1200	0.97762
1500	0.98676
1800	0.98041
2400	0.97161

[a] *current and initial radical concentrations ratio.*

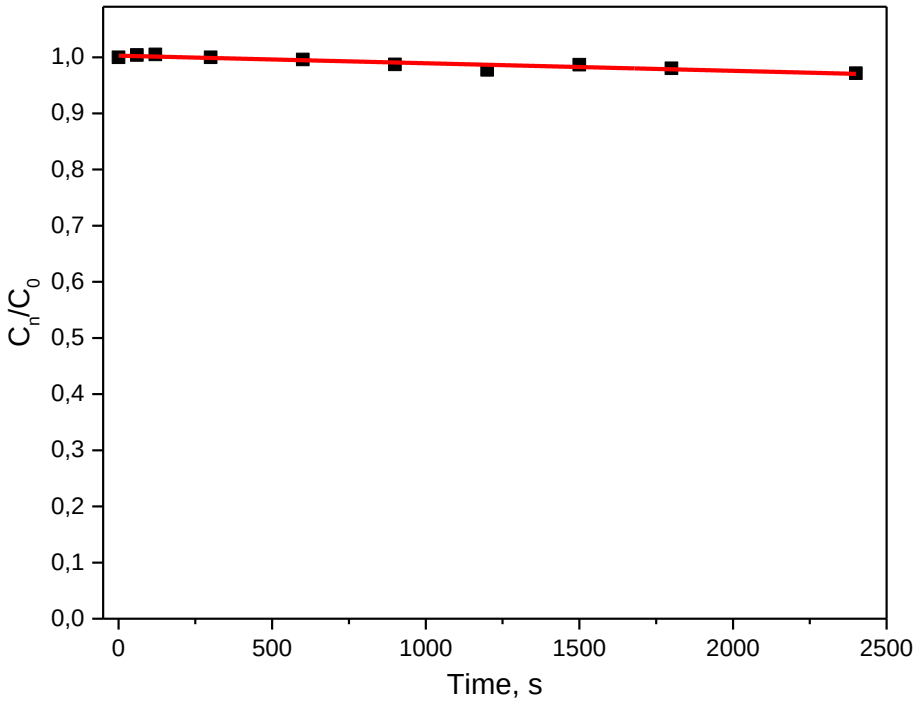


Figure S3.2. Experimental points and fitted curve for zero order decomposition reaction of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** using 405 nm LED (76 mW power, 1.562·1017 photons per second). R^2=0.86936; k_3=1.349E-5 s^{-1} (standard error 1.728E-6 s^{-1}).

Table S3.3. Decomposition of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	C_n/C_0[a]
0	1.00000
600	0.99595
1200	0.99854
1800	0.99073
2400	0.98685
3000	0.97309
3600	0.97424
4800	0.96692
6000	0.95203
7200	0.94454

[a] *current and initial radical concentrations ratio.*

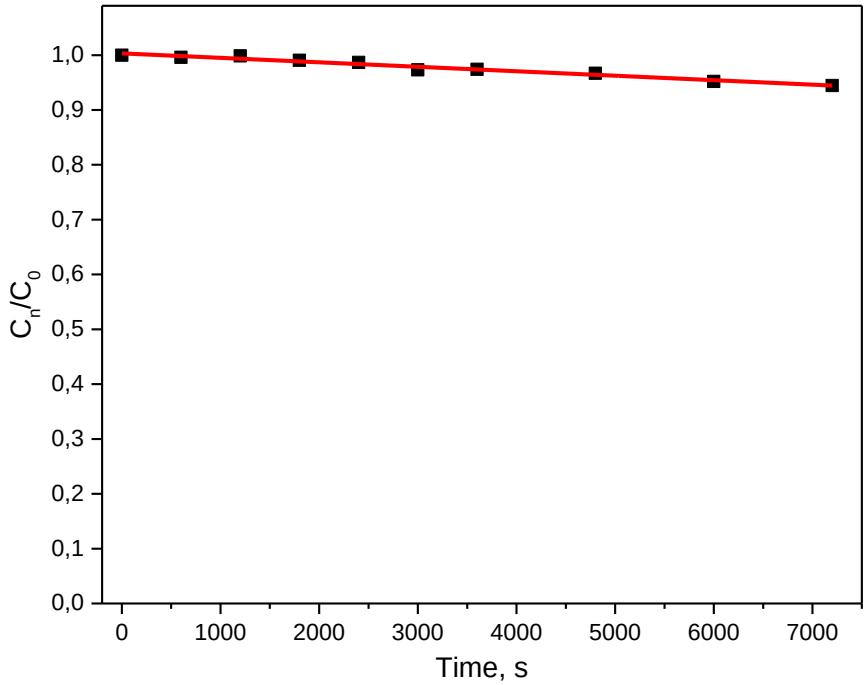


Figure S3.3. Experimental points and fitted curve for zero order decomposition reaction of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.96628; k_3=8.148E-6 s^{-1} (standard error 5.064E-7 s^{-1}).

Table S3.4. Decomposition of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** using 530 nm LED (58 mW power, $1.562 \cdot 10^{17}$ photons per second photons per second).

Time, s	C_n/C_0[a]
0	1.00000
3600	1.03722
7200	1.03048
10800	1.03292
14400	1.01728
18000	0.99349

[a] *current and initial radical concentrations ratio.*

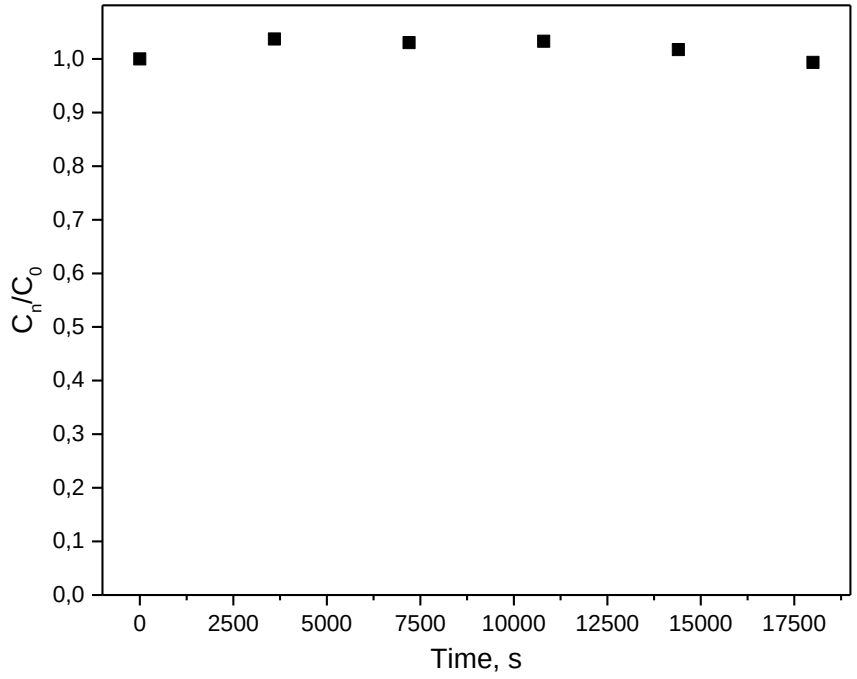


Figure S3.4. Experimental points demonstrating the absence of 1,5-diphenyl-3-(4-nitrophenyl)-6-oxoverdazyl radical **15** decay under 530 nm LED (58 mW power, $1.562 \cdot 10^{17}$ photons per second) irradiation. Fitting was not converged since no decomposition was observed.

1,3,5-triphenyl-6-oxoverdazyl radical 16

Table S3.5. Decomposition of 1,3,5-triphenyl-6-oxoverdazyl radical **16** using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	C_n/C_0[a]
0	1.00000
30	1.00531
60	1.00770
120	1.01386
300	0.99979
600	0.98924
900	1.00299
1200	0.99633
2100	0.98065

[a] *current and initial radical concentrations ratio.*

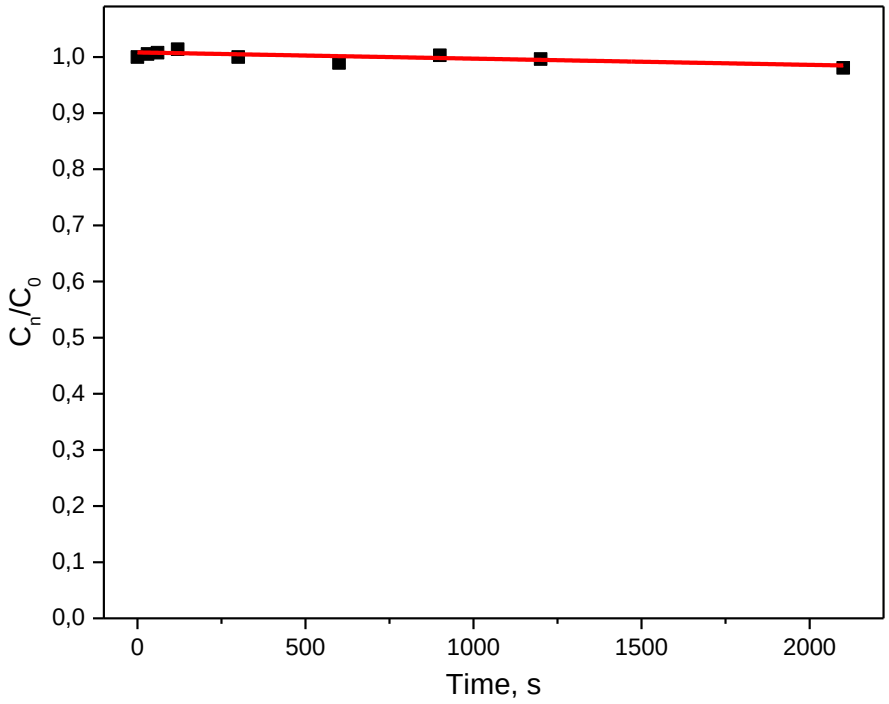


Figure S3.5. Experimental points and fitted curve for zero order decomposition reaction of 1,3,5-triphenyl-6-oxoverdazyl radical **16** using 365 nm LED (85 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.56222; k_3=1.105E-5 s^{-1} (standard error 3.290E-6 s^{-1}).

Table S3.6. Decomposition of 1,3,5-triphenyl-6-oxoverdazyl radical **16** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	C_n/C_0[a]
0	1.00000
30	0.99216
60	1.00162
300	0.97966
600	0.97464
900	0.97255
1200	0.94522
2400	0.96830

[a] *current and initial radical concentrations ratio.*

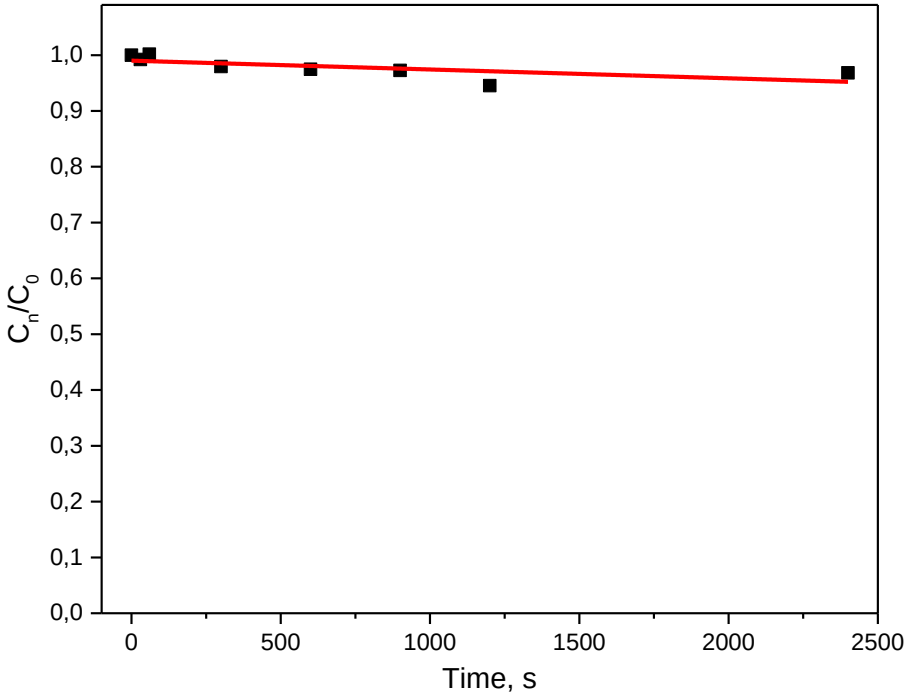


Figure S3.6. Experimental points and fitted curve for zero order decomposition reaction of 1,3,5-triphenyl-6-oxoverdazyl radical **16** using 405 nm LED (76 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.39273; k_3=1.579E-5 s^{-1} (standard error 6.716E-6 s^{-1}).

Table S3.7. Decomposition of 1,3,5-triphenyl-6-oxoverdazyl radical **16** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second).

Time, s	C_n/C_0[a]
0	1.00000
300	0.99432
600	0.99418
1200	0.99401
2400	0.99620
3600	0.99124
5400	0.98853
7200	0.98802
9000	0.98209

[a] *current and initial radical concentrations ratio.*

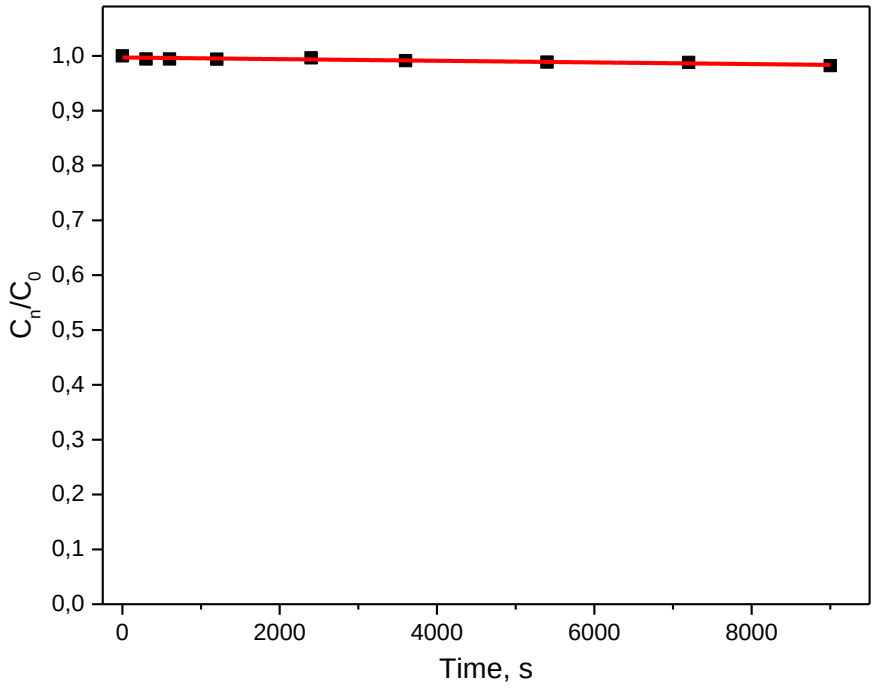


Figure S3.7. Experimental points and fitted curve for zero order decomposition reaction of 1,3,5-triphenyl-6-oxoverdazyl radical **16** using 455 nm LED (68 mW power, $1.562 \cdot 10^{17}$ photons per second). R^2=0.83307; k_3=1.498E-6 s^{-1} (standard error 2.342E-7 s^{-1}).

Section S4. Experimental and Theoretical UV-Vis Spectra. Natural Transition Orbitals and Cartesian Coordinates of AlkVZs 1 – 8

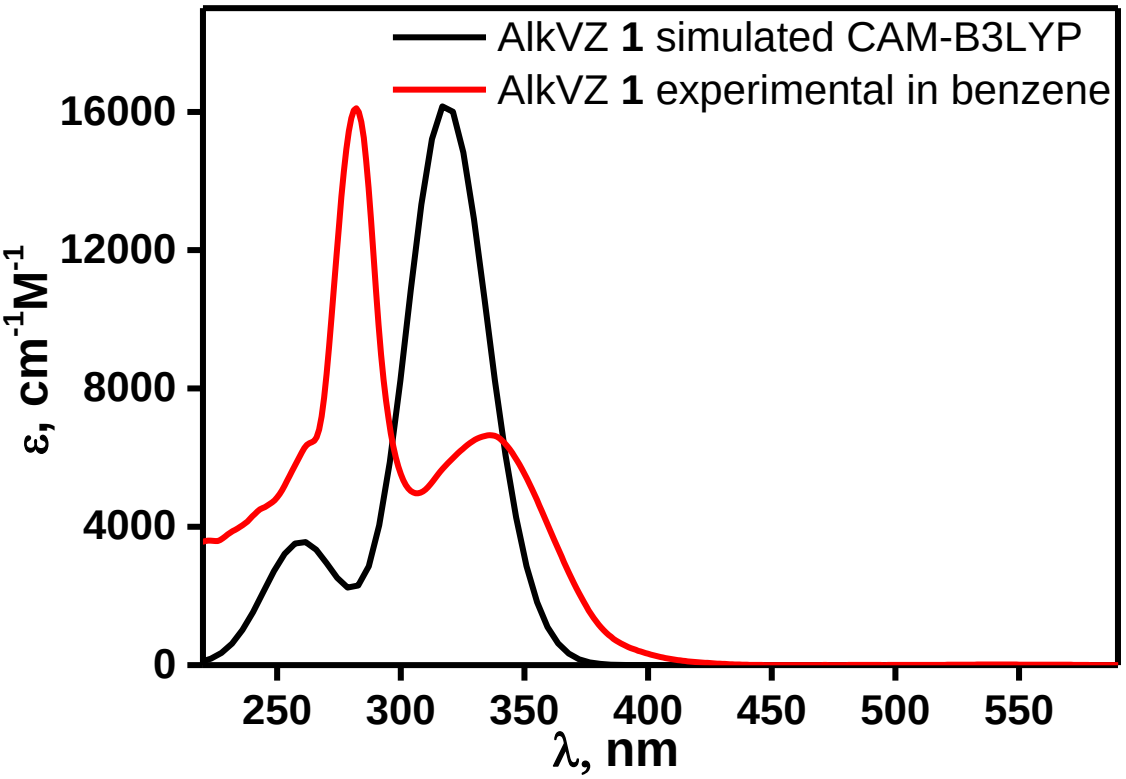


Figure S4.1. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **1**.

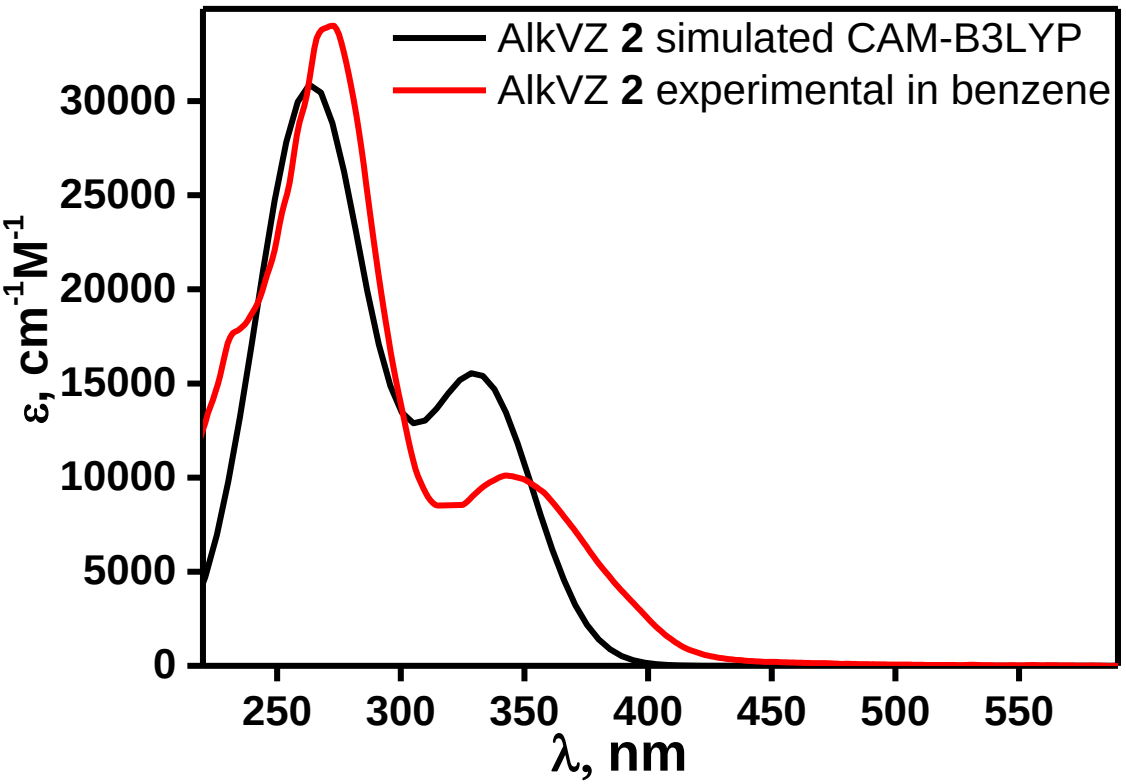


Figure S4.2. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **2**.

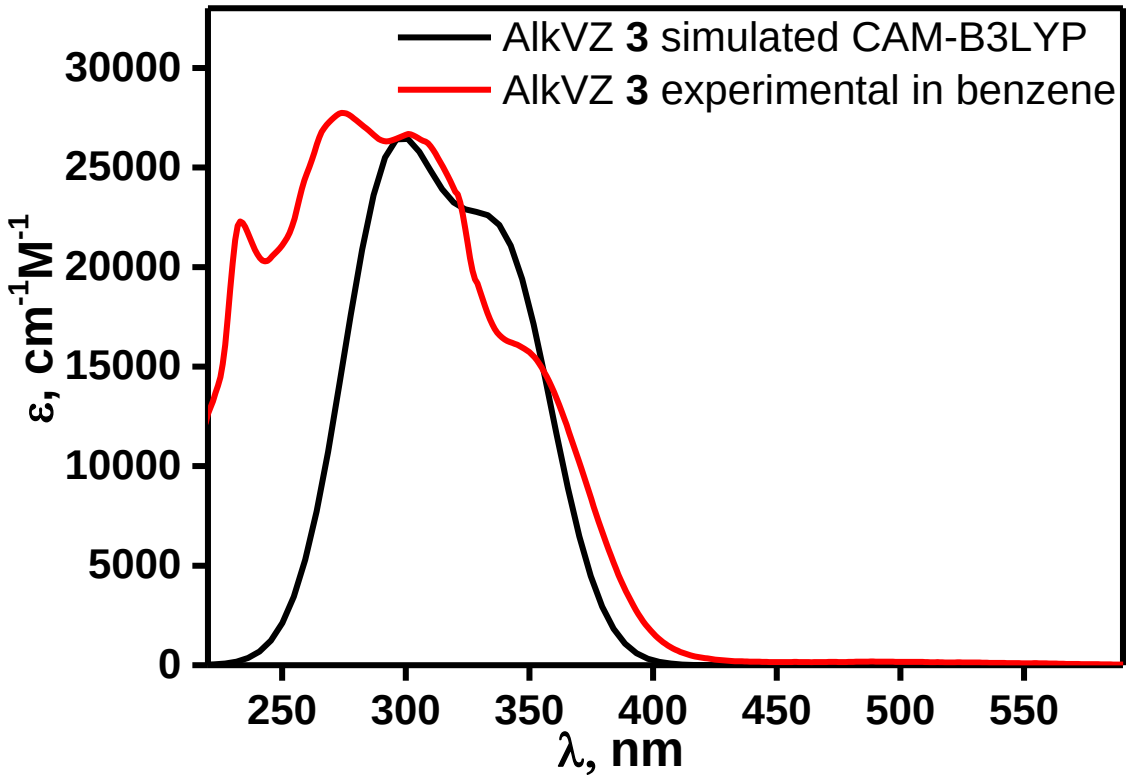


Figure S4.3. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **3**.

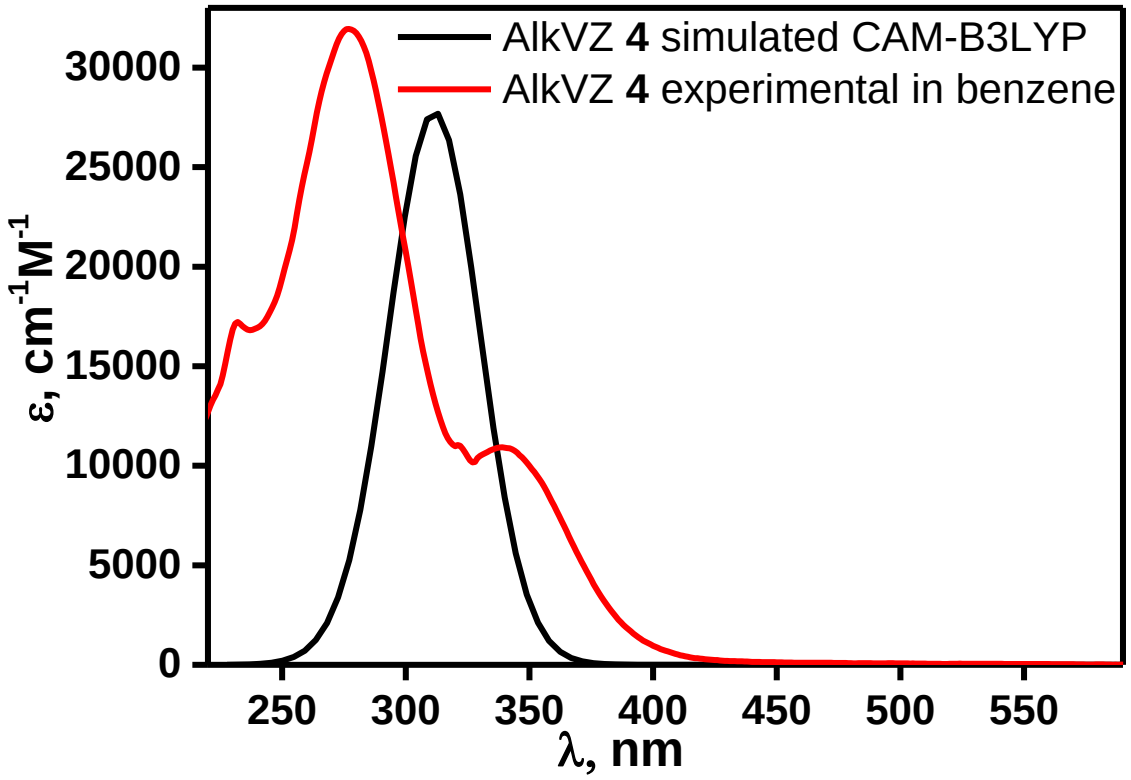


Figure S4.4. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **4**.

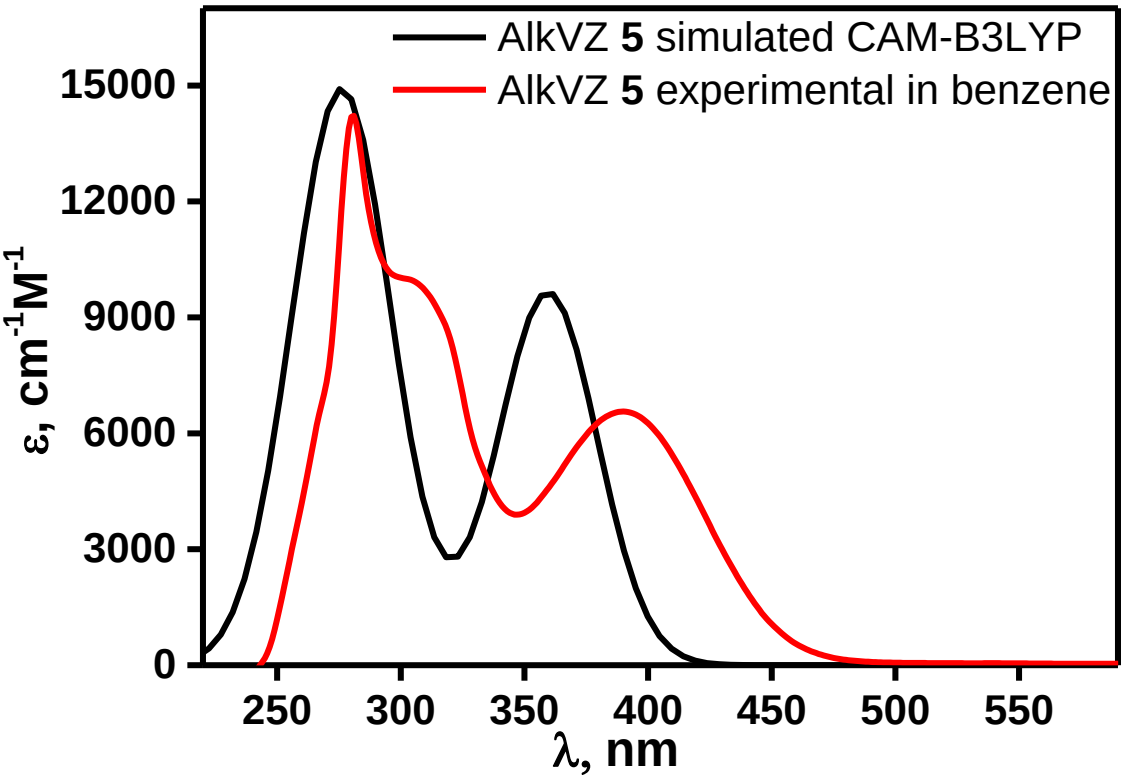


Figure S4.5. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **5**.

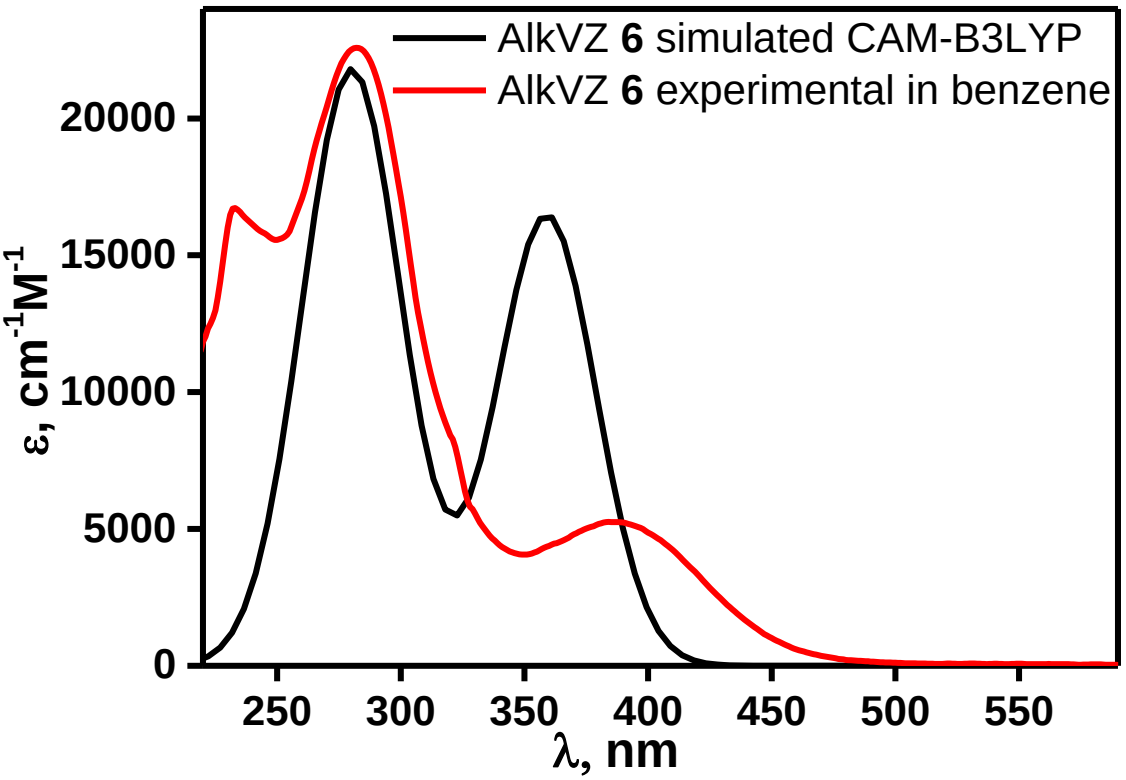


Figure S4.6. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **6**.

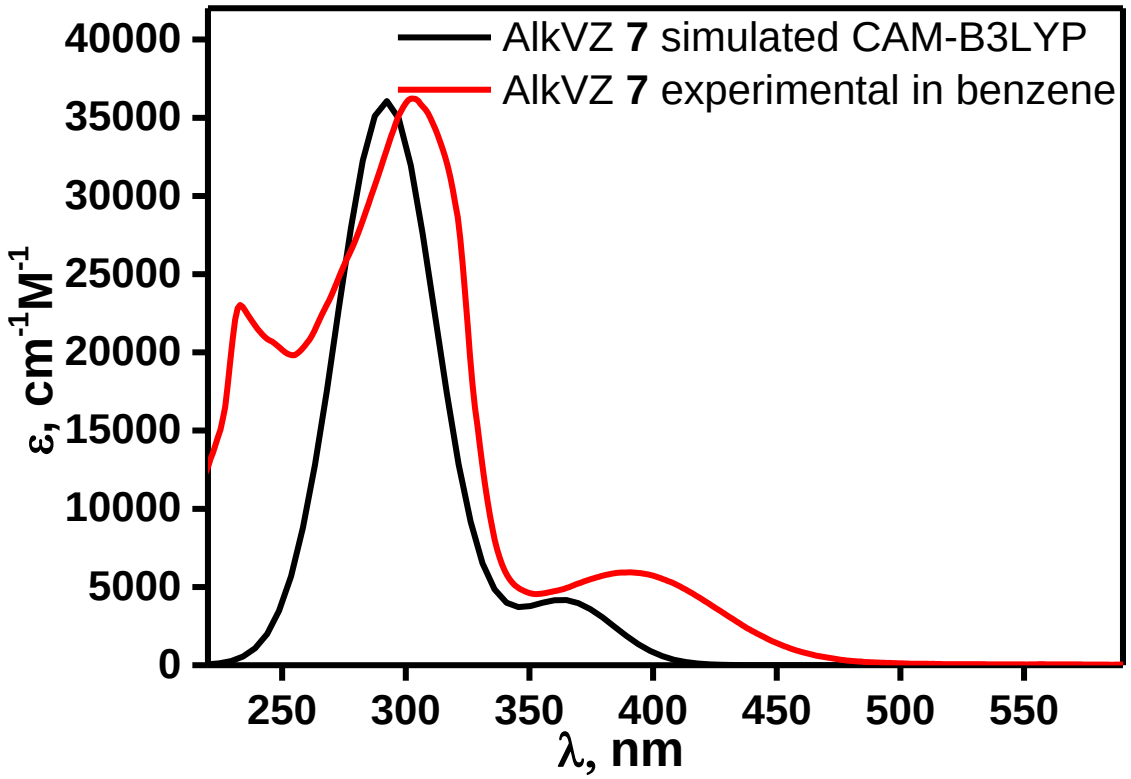


Figure S4.7. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **7**.

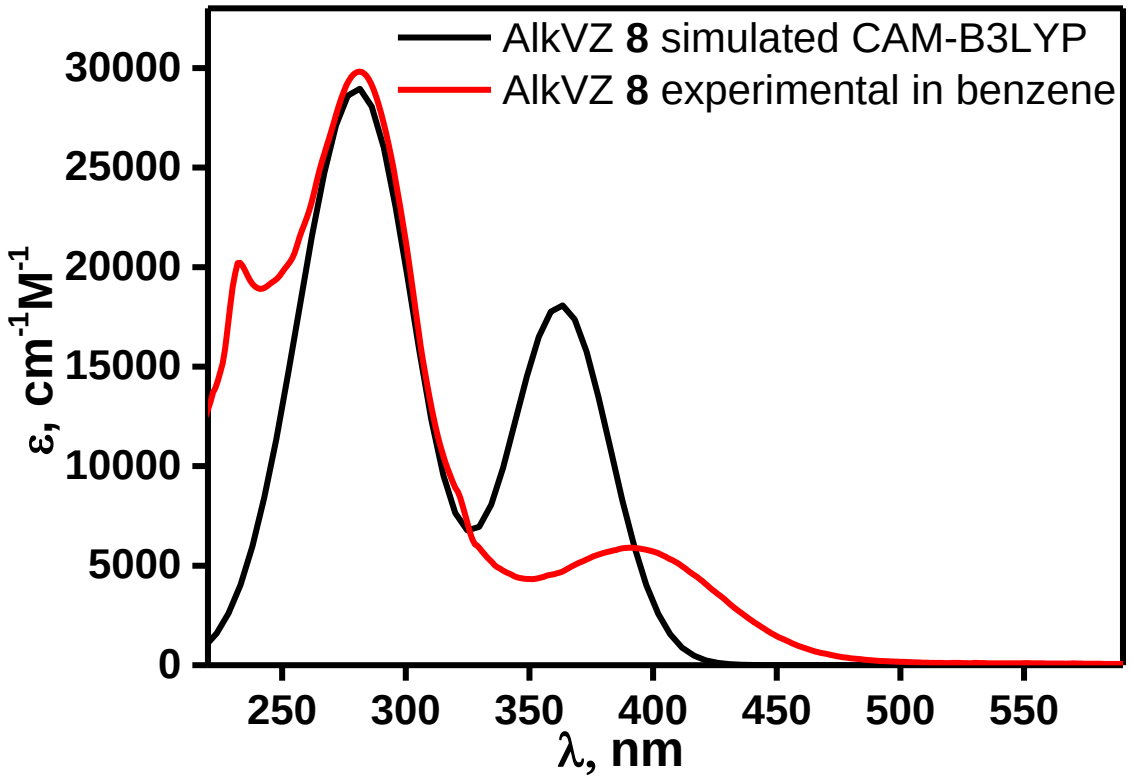


Figure S4.8. Experimental (10^{-4} M in benzene) and simulated (CAM-B3LYP) UV-Vis spectra of AlkVZ **8**.

Table S4.1. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **1** for $S_1 - S_5$ excited states.

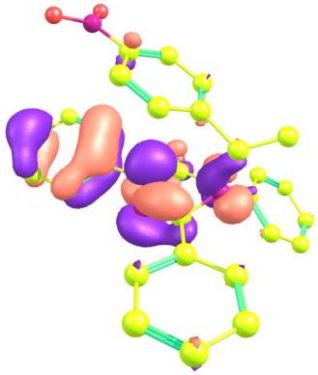
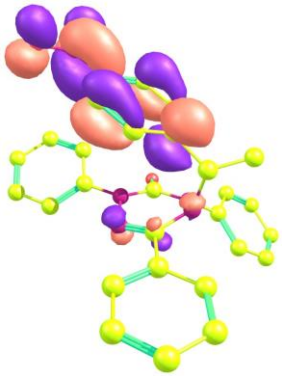
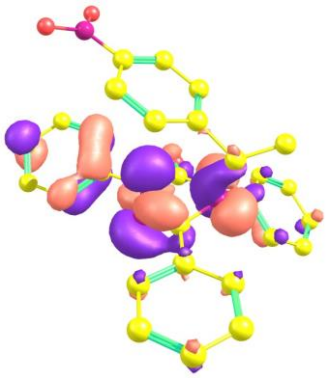
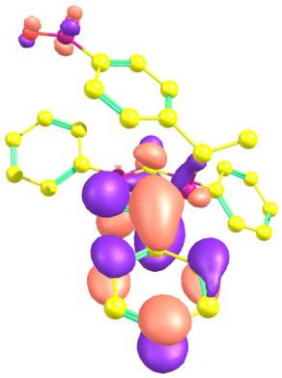
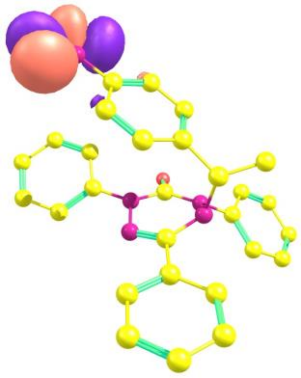
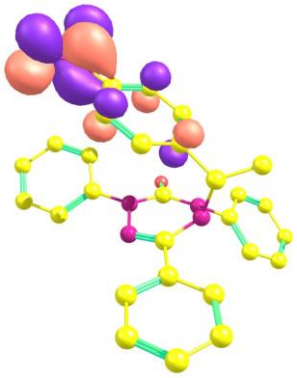
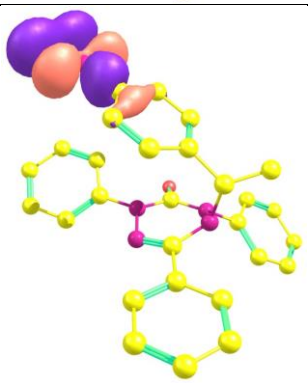
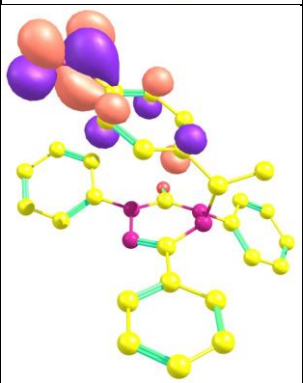
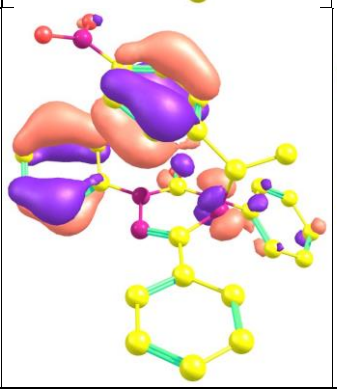
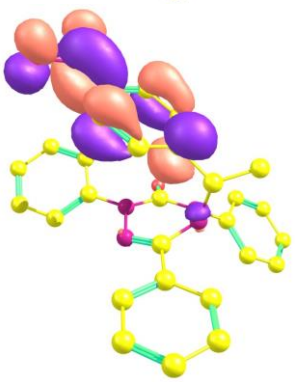
Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			+	335	0.030204
$S_0 - S_2$			±	317	0.146962
$S_0 - S_3$			-	311	0.000745
$S_0 - S_4$			-	278	0.000275
$S_0 - S_5$			±	260	0.035489

Table S4.2. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **2** for $S_1 - S_5$ excited states.

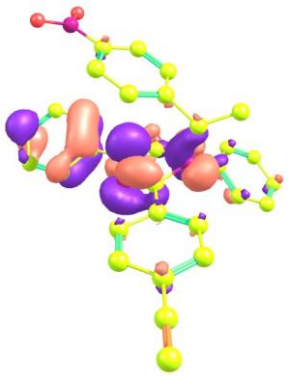
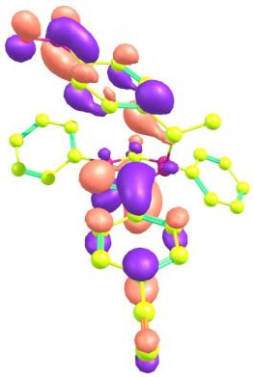
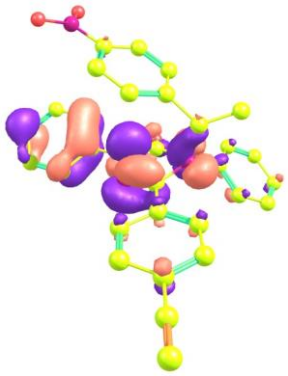
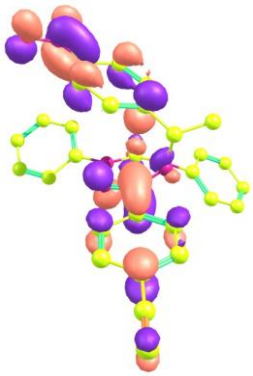
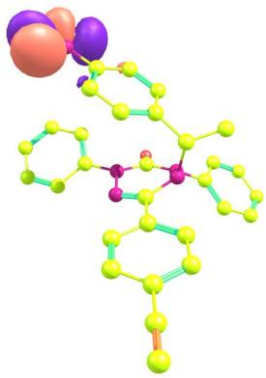
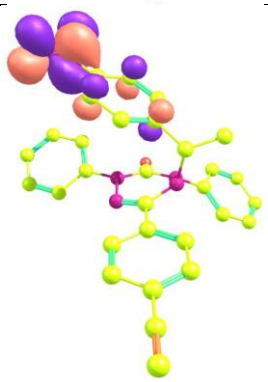
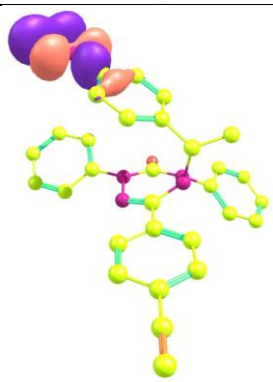
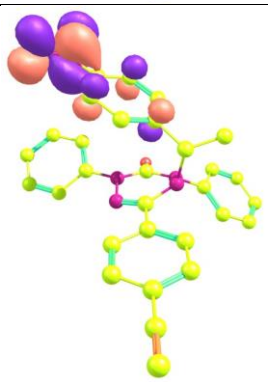
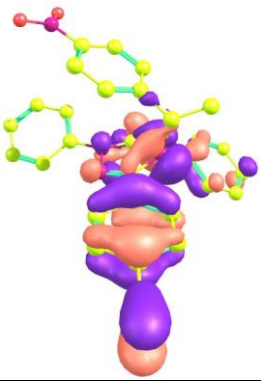
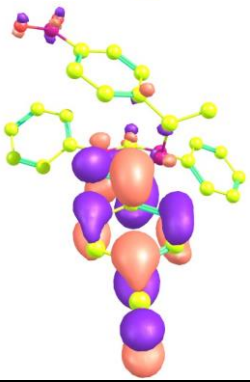
Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			±	336	0.1281711
$S_0 - S_2$			±	328	0.181181
$S_0 - S_3$			-	311	0.000796
$S_0 - S_4$			-	278	0.000297
$S_0 - S_5$			±	264	0.614305

Table S4.3. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **3** for $S_1 - S_5$ excited states.

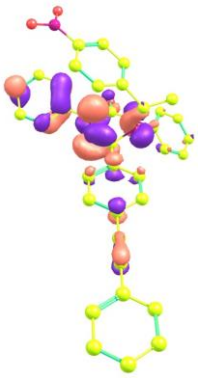
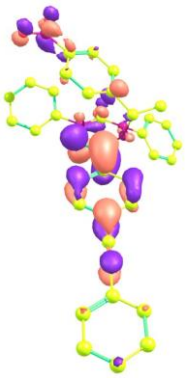
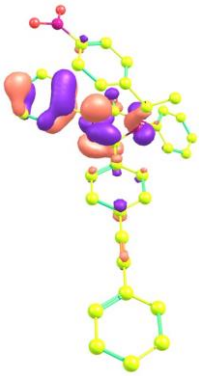
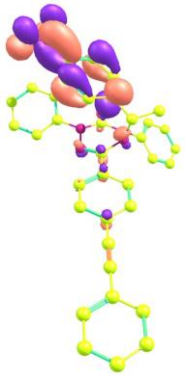
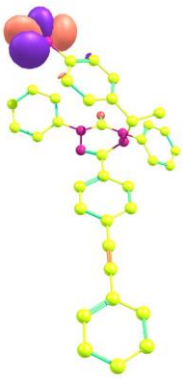
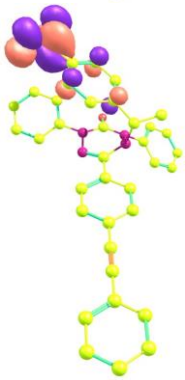
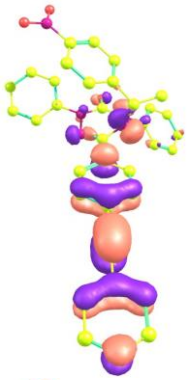
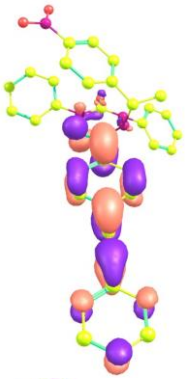
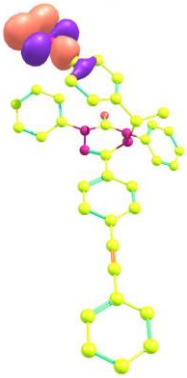
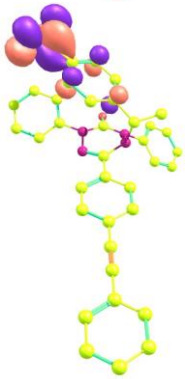
Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			±	342	0.6035832
$S_0 - S_2$			+	334	0.265093
$S_0 - S_3$			-	311	0.001156
$S_0 - S_4$			-	294	1.052564
$S_0 - S_5$			-	278	0.000313

Table S4.4. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **4** for S_1 – S_5 excited states.

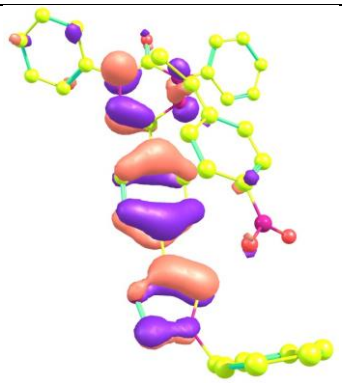
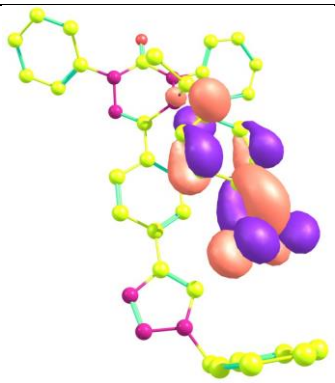
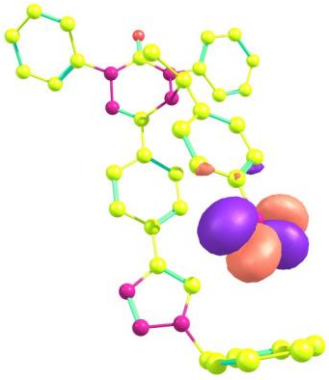
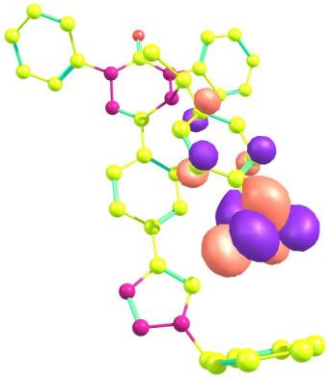
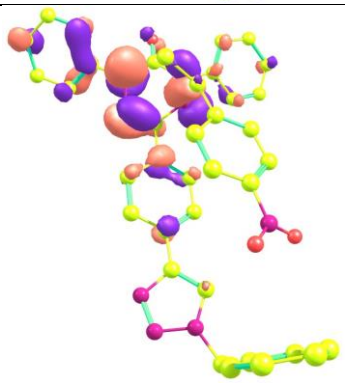
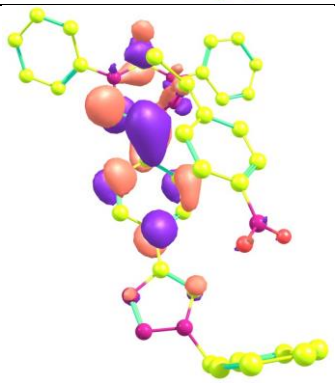
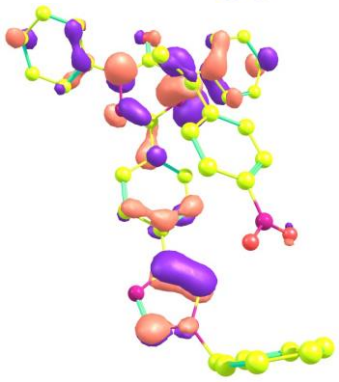
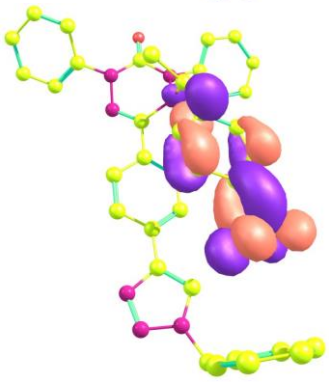
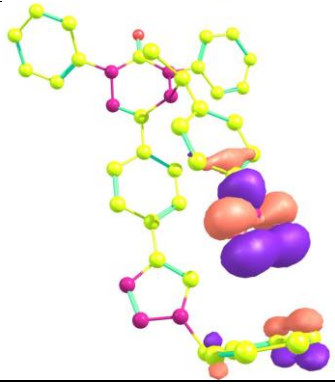
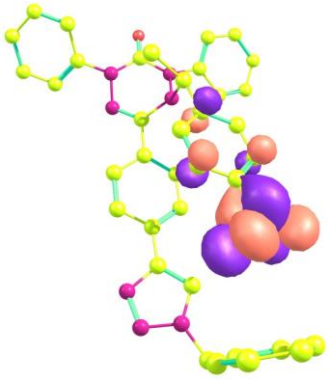
Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			+	341	0.0035
$S_0 - S_2$			-	313	0.0364
$S_0 - S_3$			-	312	0.3692
$S_0 - S_4$			+	290	0.0216
$S_0 - S_5$			-	282	0.0002

Table S4.5. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **5** for $S_1 - S_5$ excited states.

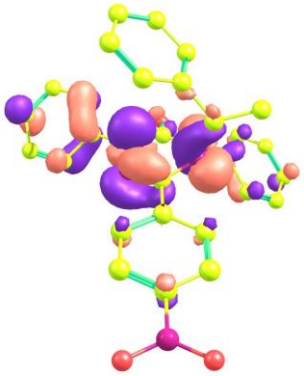
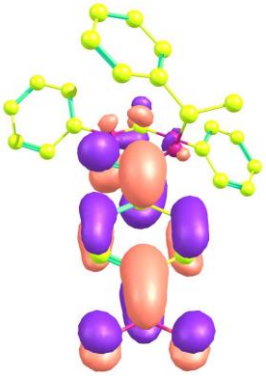
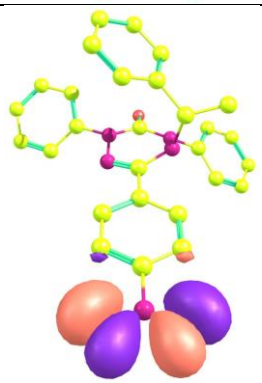
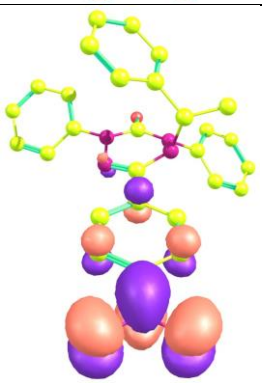
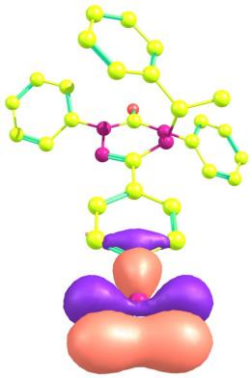
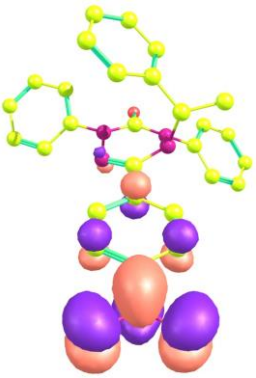
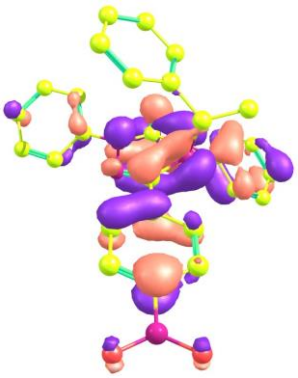
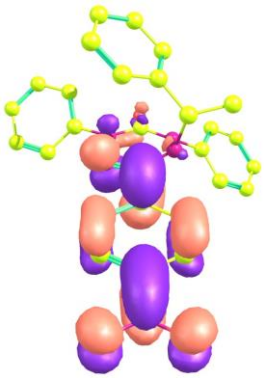
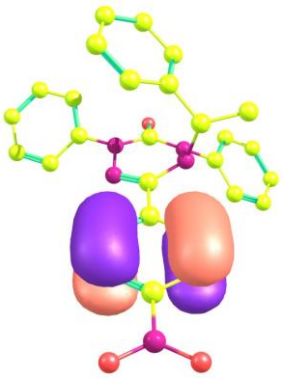
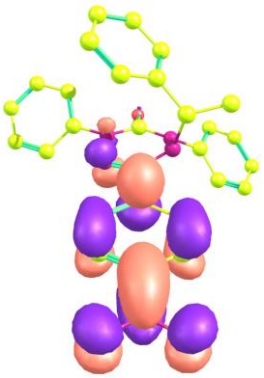
Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			±	360	0.2412788
$S_0 - S_2$			-	314	0.000464
$S_0 - S_3$			-	280	0.00235
$S_0 - S_4$			±	276	0.362999
$S_0 - S_5$			-	263	0.009368

Table S4.6. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **6** for $S_1 - S_5$ excited states.

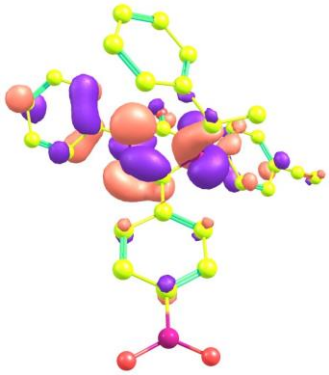
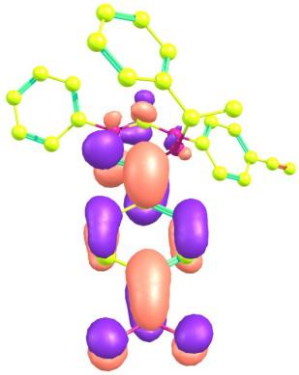
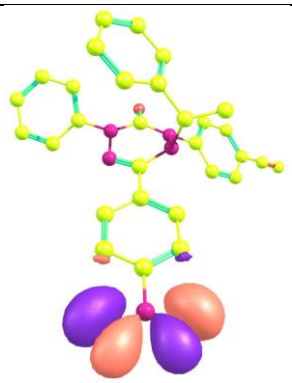
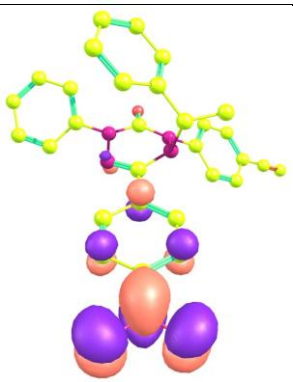
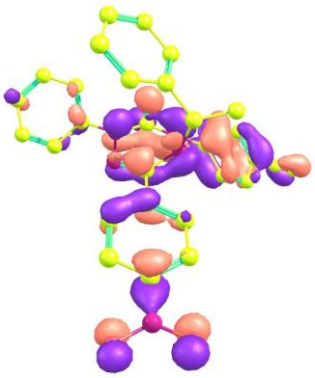
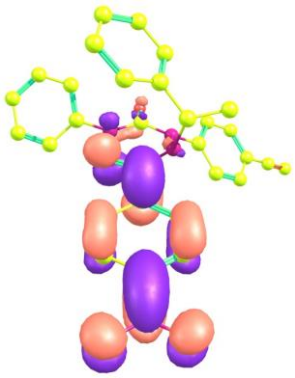
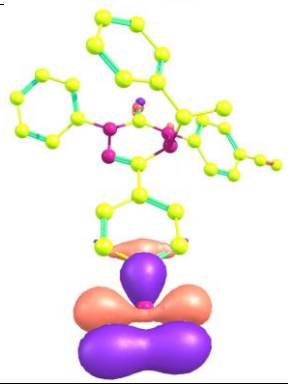
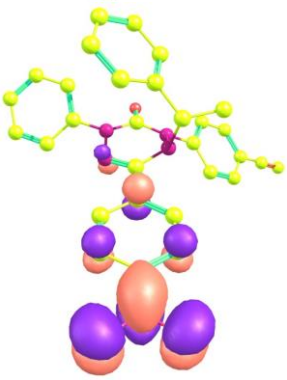
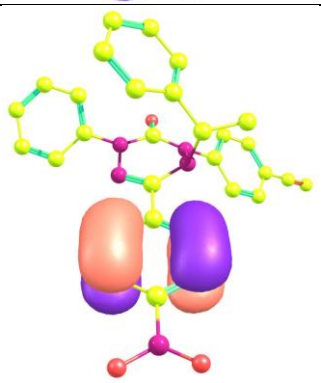
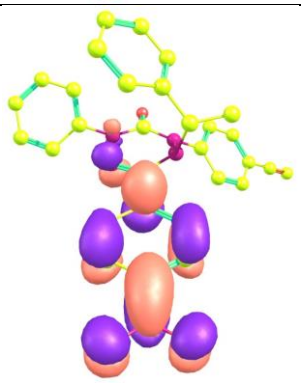
Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			±	359	0.2305
$S_0 - S_2$			-	314	0.0005
$S_0 - S_3$			±	280	0.2648
$S_0 - S_4$			-	280	0.0381
$S_0 - S_5$			-	263	0.0031

Table S4.7. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **7** for $S_1 - S_5$ excited states.

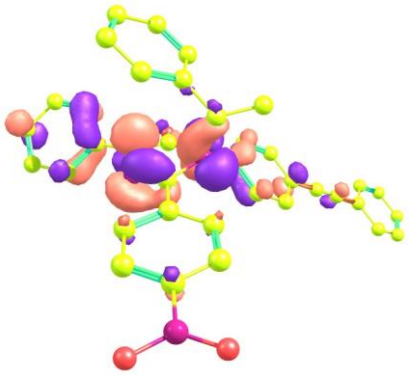
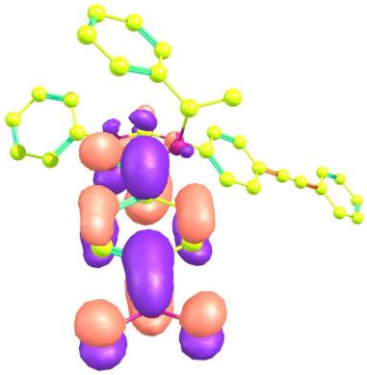
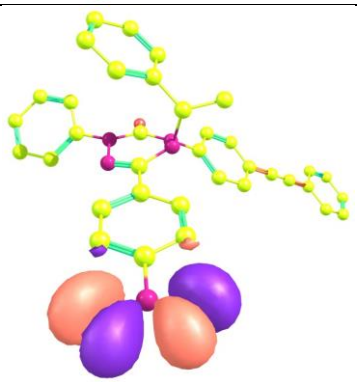
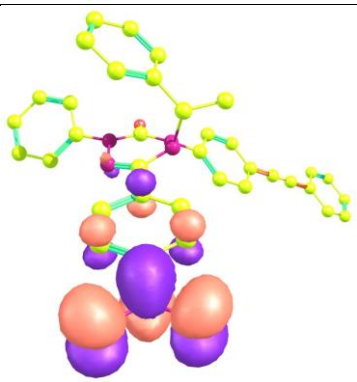
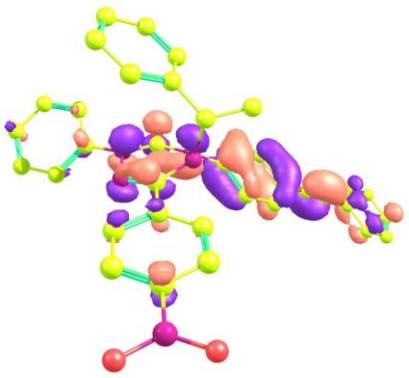
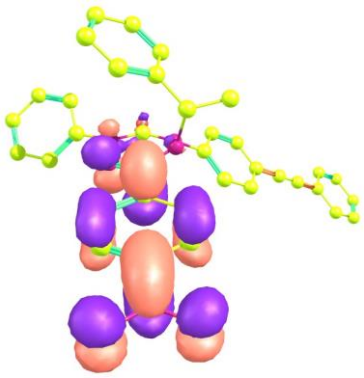
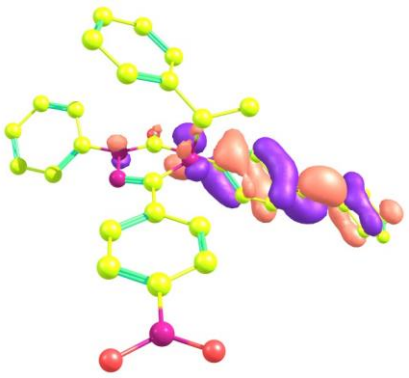
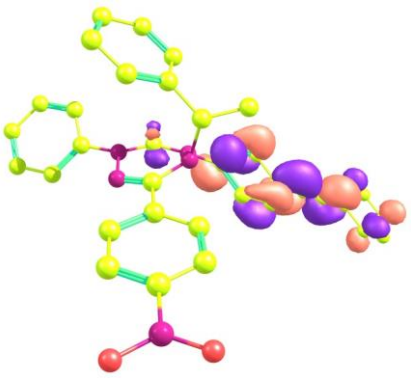
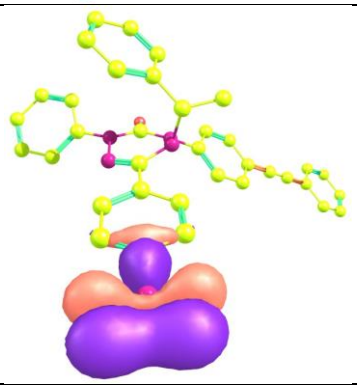
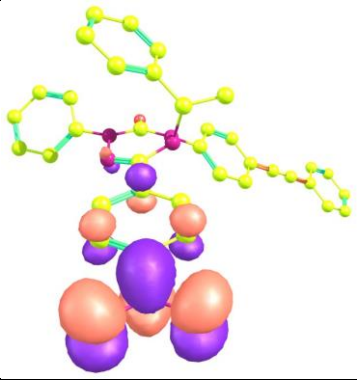
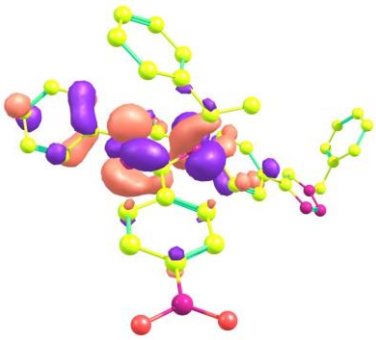
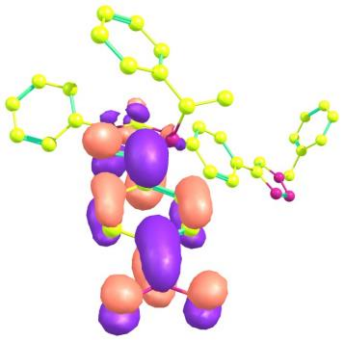
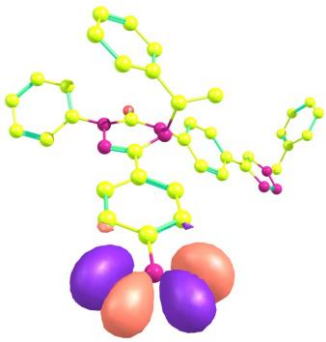
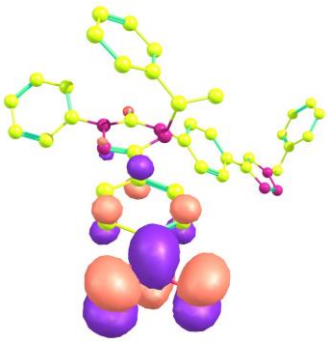
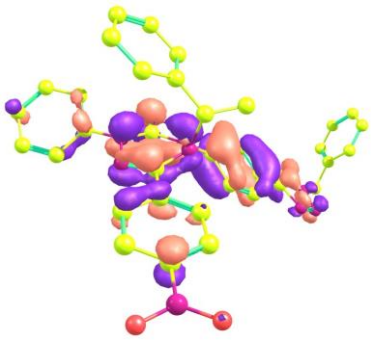
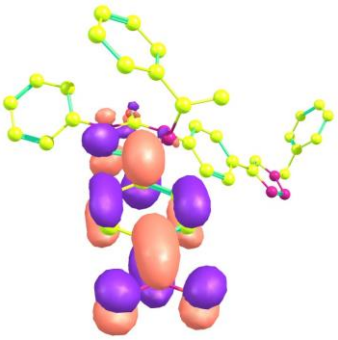
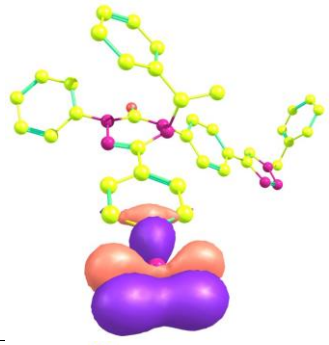
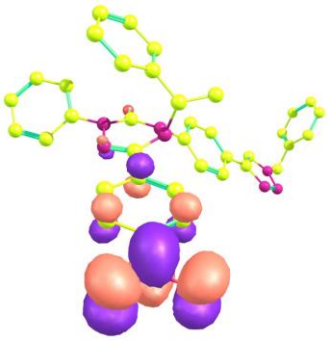
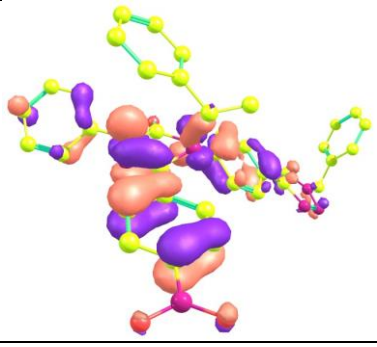
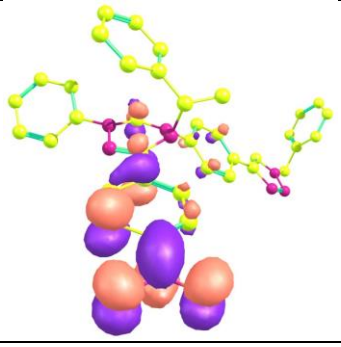
Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			±	364	0.2140
$S_0 - S_2$			-	314	0.0008
$S_0 - S_3$			-	295	0.2691
$S_0 - S_4$			±	292	1.6091
$S_0 - S_5$			-	280	0.0003

Table S4.8. Calculated NTOs, wavelengths (λ) and oscillator strengths (f) of AlkVZ **8** for $S_1 - S_5$ excited states.

Transition	"Partical" orbital	"Hole" orbital	Charge separation	λ, nm	f
$S_0 - S_1$			±	363	0.2169
$S_0 - S_2$			-	314	0.0007
$S_0 - S_3$			-	287	0.2607
$S_0 - S_4$			-	280	0.0007
$S_0 - S_5$			±	260	0.0355

The Cartesian coordinated of atoms for the considered molecules in ground electronic state obtained on CAM-B3LYP/def2-TZVP level of theory

AlkVZ 1

C	-1.388577126510	-2.682145287029	1.967246375978
C	-1.356027832747	-3.800143756339	2.792646087151
C	-0.331695983887	-3.956536579048	3.720353400900
C	0.668168487470	-2.988842280331	3.815800761140
C	0.646774827754	-1.874830079961	2.991336706206
C	-0.389456676837	-1.705164394508	2.061337311475
C	-0.407841458014	-0.529457752077	1.182803671196
N	-1.217880544547	-0.584668932115	0.024274959681
N	-1.652648982663	0.690687629525	-0.378196988890
C	-0.794844588202	1.786285162055	-0.264944057543
N	0.322977563058	1.512531880768	0.535356559457
N	0.309505516590	0.499153765380	1.468518877877
C	1.392502356149	2.449261477719	0.668236901696
C	-0.650112232755	-1.421386896437	-1.094823028853
O	-1.022328683149	2.873362008575	-0.757310063770
C	0.604157706345	-0.778802828483	-1.643198714987
C	-1.730815258622	-1.720005605325	-2.120893013434
C	0.558709850802	0.156820389956	-2.682087249837
C	1.700087317371	0.847154101970	-3.062374516333
C	-3.062121209820	0.854901450249	-0.554467135554
C	2.891312490714	0.586840662571	-2.397756660011
C	2.979315286153	-0.362173427183	-1.388143630342
C	1.829229195268	-1.043622411281	-1.020459403997
C	2.055006255938	2.579699351713	1.888734885853
C	3.148298603650	3.433513525346	1.988035025469
C	3.589825023465	4.154798700027	0.884720696642
C	2.919142734256	4.021824973953	-0.328022918841
C	1.822900465419	3.177837393556	-0.442855778100
C	-3.941823008644	0.135636393932	0.255698477111
C	-5.312171953466	0.267020676919	0.071376111958
C	-5.814660186637	1.116480769610	-0.910482950468
C	-4.930940671304	1.833116789310	-1.710354840049
C	-3.555816040864	1.702899766339	-1.546714299840
N	4.088725984853	1.369399638724	-2.749019010904
O	3.947591121307	2.292538898550	-3.543681383320
O	5.147243197456	1.058370986488	-2.217919639401
H	-2.194598354869	-2.556400255732	1.250670570659
H	-2.138302440197	-4.549297579662	2.713886370057
H	1.474012414050	-3.109992694939	4.533756233192
H	1.427646482243	-1.123657828654	3.051919022390
H	-0.363428058591	-2.357769993724	-0.599260611640
H	-2.144821884857	-0.809535023716	-2.561483042668
H	-1.313846552256	-2.332703001148	-2.925760723975
H	-2.555500895818	-2.263148988239	-1.650922961991
H	-0.377315315349	0.368117717741	-3.188856447251
H	1.676212186653	1.591980681672	-3.849068687210
H	3.928999003364	-0.540681669990	-0.898327994381
H	1.875604010289	-1.777534500753	-0.219601272872
H	1.719517682787	2.010802126740	2.747039177563
H	3.658035908719	3.529950626189	2.942279483095
H	4.449417423269	4.812712230782	0.965962333013

H	3.254510801231	4.571237414487	-1.202670113830
H	1.308367711354	3.082487263210	-1.389904679031
H	-3.549988610714	-0.516539012121	1.028667844465
H	-5.990721750578	-0.290593358982	0.710440293380
H	-6.886462130131	1.218945194794	-1.049533889907
H	-5.310367392029	2.497973684542	-2.480759353922
H	-2.867786823840	2.260820138699	-2.169021064253
H	-0.308099955005	-4.829712105451	4.365568175008

AlkVZ 2

C	-2.600863785249	-1.409168189302	2.091676308520
C	-3.773275712269	-2.078659784409	2.381868207867
C	-4.821362592117	-2.126587604344	1.443699951276
C	-4.654966081830	-1.480795793057	0.209062374214
C	-3.480228431315	-0.805044182793	-0.076497032071
C	-2.438461486900	-0.755194549307	0.859947601131
C	-1.189332508781	-0.054406054004	0.554012158864
C	-6.022354807522	-2.818675413985	1.740635287856
N	-0.920801516896	0.256375943948	-0.799996762296
N	-0.101177981950	1.392773590424	-0.927046471602
C	0.930760141924	1.614786867687	-0.015465717834
N	0.825425568917	0.802977283585	1.125334654490
N	-0.371320317260	0.242454592422	1.502594882425
C	1.839413927583	0.810130650045	2.131969316689
C	-0.470692107857	-0.920985091100	-1.630569752543
O	1.791089127767	2.459470266442	-0.160575300068
C	-7.043037871230	-3.409835815234	1.997509989450
C	0.892050498378	-1.391867108918	-1.175962356072
C	-0.584388437354	-0.589730187185	-3.109774815107
C	0.977255776313	-2.308011787135	-0.121629197948
C	2.203216049362	-2.655883893686	0.424737123732
C	-0.571819503000	2.422558890786	-1.799911721130
C	3.350085095797	-2.077982705119	-0.102916021770
C	3.304651563850	-1.192240149432	-1.171656453969
C	2.069994594624	-0.855908273573	-1.707052004932
C	3.185183584914	0.820874627391	1.761659039727
C	4.166536902986	0.748936344853	2.741094881442
C	3.821337795684	0.671244691268	4.087631374057
C	2.478394423242	0.669047665962	4.447113627863
C	1.483288872244	0.736690874344	3.477912472720
C	-1.944384887105	2.648222655676	-1.913167619373
C	-2.412639853451	3.624957821291	-2.782470475695
C	-1.522729334467	4.385688943485	-3.535721304155
C	-0.156355483172	4.157305555190	-3.413311039315
C	0.327938923327	3.174008161027	-2.556913234854
N	4.652414420428	-2.384422504522	0.514348204694
O	5.625422269747	-1.747239303804	0.126231240064
O	4.680472975815	-3.246056859070	1.383643597594
H	-1.790649330637	-1.382946776952	2.812959883814
H	-3.895361551154	-2.582365672785	3.335166450245
H	-5.460070394220	-1.511470725179	-0.517673498895
H	-3.366185410410	-0.299435983237	-1.030429388038
H	-1.199307406055	-1.704470445272	-1.386070635519
H	-7.944244217735	-3.927618657240	2.222353354091
H	-1.619567368427	-0.341960071956	-3.360481017107
H	0.035972187947	0.264602857085	-3.392194916869
H	-0.271282994442	-1.453280580354	-3.704179857772
H	0.067661077720	-2.737917267066	0.290745312266
H	2.282073259656	-3.347961495337	1.254503171851
H	4.224018786269	-0.767210776461	-1.556883056241
H	2.027142181789	-0.152572352299	-2.532293544425
H	3.463140557073	0.882705070713	0.717564135422
H	5.210379876575	0.744436145737	2.441765122718
H	4.593619459038	0.610575602942	4.848073823961

H	2.193929048441	0.613761852601	5.493855915793
H	0.437098061511	0.725821467194	3.758446427108
H	-2.636845993606	2.062684343173	-1.318136512251
H	-3.481839520690	3.799304951982	-2.860564470412
H	-1.892367925127	5.150278863362	-4.211937579213
H	0.548045430472	4.742794599390	-3.996883183321
H	1.391490363131	2.995991891563	-2.462423953115

AlkVZ 3

C	1.454259226655	-0.974308016512	1.997454000922
C	2.516182379109	-1.500329956051	2.712021112205
C	2.468427291352	-2.819501670223	3.196712261129
C	1.314904273992	-3.589735749554	2.941659600584
C	0.255848678153	-3.059403411765	2.233691606447
C	0.309969993533	-1.744184637588	1.743290713205
C	-0.821883548511	-1.182414227533	1.005411112505
C	3.547941262525	-3.359612188995	3.926165261816
N	-0.885549262321	0.224260510599	0.865424040679
N	-1.577642600378	0.608897923886	-0.296989078215
C	-2.696869867840	-0.114302636813	-0.713002578455
N	-2.813801093523	-1.348831495387	-0.056869468475
N	-1.727616060092	-1.961267463285	0.524413580011
C	-3.954791307223	-2.186515601248	-0.249657618020
C	-1.321489909260	0.955152150192	2.111005613555
O	-3.452189518169	0.256649962176	-1.588814107701
C	4.475966918347	-3.827171730182	4.555011588849
C	-2.759201448034	0.618936177522	2.436553958028
C	-1.010175255901	2.437106731600	1.980054229676
C	-3.825742298973	1.355974500439	1.911231085371
C	-5.134357548296	0.932214833357	2.089869599229
C	-0.890832984687	1.501539498895	-1.178420852996
C	-5.367147590907	-0.234327799939	2.806626820427
C	-4.334574846271	-0.967669350632	3.375384148256
C	-3.032456878248	-0.529781228886	3.187810543674
C	-5.229713904239	-1.621168690377	-0.318728950625
C	-6.341530498341	-2.446092169840	-0.422247940550
C	-6.197761716000	-3.830186003373	-0.464048887583
C	-4.923843378366	-4.383716368529	-0.403846651073
C	-3.800045676439	-3.571705372236	-0.295007130928
C	-1.596975279029	2.463482946210	-1.901791372196
C	-0.904294918855	3.329917553937	-2.741117398639
C	0.480131418669	3.259471891894	-2.852415175269
C	1.176401011198	2.301910098269	-2.120028222588
C	0.498217350862	1.421024429533	-1.287503539950
N	-6.748513552670	-0.729557904104	2.932528365103
O	-6.941222826869	-1.699295526694	3.654703692817
O	-7.618103513266	-0.146268832862	2.294423066362
H	1.507729610581	0.042648749822	1.620898050465
H	3.400362460910	-0.900197586862	2.900394650001
H	1.267564666860	-4.606302406244	3.318366538432
H	-0.633976543305	-3.652822447337	2.050378816425
H	-0.687262264284	0.526774347564	2.897646770419
H	-1.310571506742	2.957741937039	2.894196938609
H	0.062263633086	2.582170894503	1.823075500811
H	-1.531295025898	2.895885036580	1.136005828878
H	-3.639274817242	2.258276230272	1.338043078906
H	-5.969266681098	1.479496839167	1.668256422938
H	-4.558350408879	-1.868356120736	3.934317286590
H	-2.210219378069	-1.102007693942	3.610655746801
H	-5.352503026860	-0.546614410490	-0.288204673116
H	-7.329241101622	-1.996437680499	-0.459938164490
H	-7.071745035230	-4.469511698221	-0.539992419587
H	-4.795193625386	-5.461612361311	-0.440161625332

H	-2.809123014749	-4.005168926713	-0.238317333554
H	-2.674614717725	2.518665699560	-1.815423990266
H	-1.458841671507	4.073757591677	-3.305682254993
H	1.013255623957	3.944355602155	-3.504576115055
H	2.256721678462	2.228465822992	-2.205102759855
H	1.039469553733	0.666915903725	-0.726554874416
C	5.555950930661	-4.370688078438	5.286846794198
C	5.493110025964	-5.686731761983	5.779691501170
C	6.709147254570	-3.603699533893	5.532966751625
C	6.556035224926	-6.214633123657	6.497179051680
C	7.765548312036	-4.142943439356	6.251658758332
C	7.694322535823	-5.447452170237	6.735941531932
H	4.603894945811	-6.279414421251	5.590487476770
H	6.758711774229	-2.588293147442	5.153105820560
H	6.497432772572	-7.231772100269	6.873237872121
H	8.651467508505	-3.542368141877	6.435826955531
H	8.524114722692	-5.865227588427	7.298040020320

AlkVZ 4

C	-1.479867988636	-3.944883048646	2.694205177350
C	-0.544470150407	-4.959831535875	2.792663901261
C	0.542578125258	-5.015564968214	1.907507692474
C	0.619182514813	-4.069380920614	0.877541596173
C	-0.310068067950	-3.049736939597	0.785276627429
C	-1.353426894494	-2.952641129878	1.712289995721
C	-2.248463160185	-1.792182016851	1.715016362310
N	-1.709645075215	-0.542647506210	1.310151291718
N	-2.716799768086	0.312565489634	0.803633500349
C	-3.987814024579	0.326766844483	1.357657666391
N	-4.218379106487	-0.775118193946	2.202009864597
N	-3.467354513142	-1.929779886841	2.100881616425
C	-5.494018585867	-0.939552593677	2.822633626300
C	-0.837308590583	0.175380149315	2.317073650847
O	-4.834355578492	1.160443813246	1.098999273324
C	0.497350593993	-0.535605388409	2.408990374185
C	-1.530874187419	0.415806429621	3.653496206986
C	1.414023960091	-0.369652239213	1.365156469902
C	2.597462185688	-1.088518445809	1.335049317628
C	-2.324985467237	1.129959313554	-0.294030648593
C	2.864435866574	-1.966318658761	2.379891115699
C	2.004144569674	-2.110210130334	3.459590634675
C	0.819090788135	-1.388413421367	3.465431292254
C	-6.133183104233	-2.178026563530	2.788561618434
C	-7.356704495281	-2.334109404963	3.430043270324
C	-7.948114179462	-1.267868438156	4.099224249460
C	-7.299657813517	-0.036363981489	4.129622933490
C	-6.072778779844	0.132860756975	3.501569904796
C	-2.725230482108	2.465081550375	-0.381051100740
C	-2.296635819780	3.237788144204	-1.455412974849
C	-1.461016925979	2.704277938562	-2.430490703939
C	-1.055580385900	1.375857781952	-2.329507481837
C	-1.483926893965	0.587808831072	-1.269910559915
N	4.069988584886	-2.806644936407	2.320200087164
O	4.396978179713	-3.412630278378	3.331215839455
O	4.662426511812	-2.869891714762	1.243727563982
H	-2.296472169185	-3.879242202391	3.406871074125
H	-0.617158477562	-5.702870079617	3.580146133966
H	1.427019020148	-4.121268512197	0.152321147018
H	-0.218138753757	-2.301908791301	0.005499210775
H	-0.646883530411	1.143816451648	1.834540319604
H	-1.866877400128	-0.518778063359	4.114342773648
H	-0.848111223196	0.918120850730	4.346432887981
H	-2.405050712501	1.057849559311	3.517077756018
H	1.171999580381	0.306613408723	0.548180949035
H	3.301925621752	-0.991957241477	0.517308383045
H	2.249186315722	-2.803932573431	4.255128250706
H	0.124944674471	-1.529192271574	4.286667335171
H	-5.668809127505	-3.007721589784	2.269098292913
H	-7.851779592327	-3.300361291291	3.398757645350
H	-8.905075355060	-1.395143259131	4.595937331311
H	-7.747295015423	0.802880932475	4.653716738055
H	-5.570816683343	1.092843706174	3.527899747160
H	-3.376597280406	2.883322849962	0.375058603844

H	-2.616163304756	4.273749324100	-1.520203390326
H	-1.127398611570	3.317033743109	-3.262237625964
H	-0.410163652501	0.942901817926	-3.088343815924
H	-1.177156318044	-0.449392223129	-1.194242579374
C	1.600476988473	-5.998280830334	2.095689833849
N	1.458521760712	-7.089234671880	2.911008574762
N	2.570938034365	-7.760730348973	2.927362875359
N	3.447150540014	-7.118356993933	2.125453729250
C	2.888687947659	-6.011970703630	1.590804812928
H	3.445270128845	-5.335614490478	0.957885010562
C	4.832748847993	-7.577020556184	2.013047375082
H	4.850762987925	-8.572078140356	2.468456039852
H	5.084101856550	-7.676482718747	0.951204640150
C	5.787013850749	-6.634281420730	2.704594643751
C	6.669738668928	-5.848997158343	1.967894800644
C	5.766131271873	-6.525084843822	4.096289198316
C	7.530127553361	-4.965697530616	2.613258161609
C	6.624082945559	-5.643660534258	4.739597051653
C	7.508687123608	-4.863089646899	3.998608108754
H	6.681755424158	-5.921012865368	0.882758932985
H	5.067111564329	-7.128712439744	4.670774232656
H	8.208919281509	-4.350705896634	2.030160695946
H	6.601948490695	-5.561847578517	5.822360726268
H	8.176332488078	-4.170714318673	4.503046230558

AlkVZ 5

C	2.437585677772	0.034453440356	-2.703221615062
C	3.278084705830	-0.347327341627	-3.737277302220
C	3.004427916879	-1.523802743511	-4.422472072504
C	1.914449680593	-2.327437691892	-4.097611211005
C	1.085567903706	-1.942993576317	-3.060509970677
C	1.331025164658	-0.753635932409	-2.354107309172
C	0.453545624091	-0.358400571430	-1.249372400530
N	3.895226852129	-1.935593372909	-5.520242589208
N	0.921677573224	0.618789985307	-0.343968961230
N	-0.136072331502	1.336293927976	0.246804948854
C	-1.318280862864	0.685334046100	0.583146856829
N	-1.436796933955	-0.578179707481	-0.033057631007
N	-0.701768495948	-0.916856822775	-1.133761972760
C	-2.608311283935	-1.366667803042	0.186490177436
C	1.945842053819	0.119016347269	0.646023211819
O	-2.197303331003	1.170745417214	1.264133316338
C	1.332231315948	-0.847761039006	1.634822627394
C	2.676615379316	1.298215922629	1.270059491366
C	0.732806835993	-0.410127128083	2.818795970190
C	0.107562997437	-1.316419833586	3.669263889318
C	-0.046809069521	2.761875102168	0.197512579806
C	0.071874399979	-2.669914407584	3.348017857734
C	0.671230274064	-3.116351000300	2.174231645797
C	1.299473319096	-2.210624208903	1.327065324850
C	-3.036012200091	-1.604988833148	1.490948778065
C	-4.158660229680	-2.393151294095	1.706208388146
C	-4.848412630741	-2.951999498788	0.633462338129
C	-4.406568090874	-2.714323207007	-0.663936630570
C	-3.288893202977	-1.920309601517	-0.895373128786
C	-0.534063454151	3.540547814645	1.248327741591
C	-0.417985355630	4.925132676017	1.181599816407
C	0.191354193871	5.538199050157	0.092289760088
C	0.682269881942	4.752171518956	-0.946624547428
C	0.563449736624	3.369366972355	-0.901090768505
O	3.625328466908	-2.976320897705	-6.108809724282
O	4.851232205569	-1.212418570836	-5.777118887666
H	2.628863772118	0.955904416620	-2.162952029237
H	4.134096730712	0.252920424028	-4.021685454155
H	1.739330205757	-3.241167349874	-4.652871182341
H	0.237454420995	-2.557774672010	-2.779331655742
H	2.653510062068	-0.441760708691	0.021535405439
H	3.157001255518	1.901540770744	0.494410828967
H	3.440612817807	0.929228173572	1.960513837989
H	2.001959463303	1.953154316937	1.826840129916
H	0.747792124947	0.643077196424	3.083088653624
H	-0.355116856567	-0.961690113383	4.585984064485
H	-0.420659576184	-3.375390027156	4.010869614207
H	0.651166695234	-4.171679830866	1.919009268732
H	1.769563721862	-2.563621762605	0.411231595558
H	-2.488602438569	-1.179536449136	2.323583508600
H	-4.491226064178	-2.577052911513	2.723548714118
H	-5.723935849456	-3.569804022792	0.808389236522
H	-4.937851136805	-3.143190648809	-1.508507166747
H	-2.940936314180	-1.730627751308	-1.904296049433

H	-1.006951449376	3.064643301406	2.097632377585
H	-0.802594790860	5.526621259447	2.000037630384
H	1.152945193864	5.217378573980	-1.807833302570
H	0.939313319628	2.758207671170	-1.714426006014
H	0.283945619361	6.619079659537	0.051997375967

AlkVZ 6

C	1.369926252521	-2.356233424416	-2.543778005282
C	2.352605700666	-3.138533009750	-3.120906525069
C	3.648090877237	-3.076139650898	-2.613883964212
C	3.979788798136	-2.249574302032	-1.548666388539
C	2.989935367432	-1.462896403088	-0.980546744070
C	1.676577102849	-1.501550423135	-1.471712054149
C	0.629492287907	-0.677061498811	-0.863168936339
N	4.696063775670	-3.913725782933	-3.222124409055
N	0.884608368573	-0.105119264833	0.403015004368
N	0.160713395338	1.087291214170	0.593566658636
C	-1.140910895385	1.197318738554	0.110289017075
N	-1.451265261815	0.201847476156	-0.836791764753
N	-0.481375818012	-0.503794947344	-1.491892239380
C	-2.740983847567	0.186980864767	-1.453436799459
C	0.785813668278	-1.069389231479	1.561229491636
O	-1.904905092285	2.093840803060	0.400957735097
C	3.174050406682	5.493940197156	2.427825384902
C	-0.645131997654	-1.493872228895	1.809602968670
C	1.502467942536	-0.493722066098	2.773702832536
C	-1.497612737678	-0.761074588715	2.639635979547
C	-2.828393068586	-1.137414002562	2.791658342005
C	0.900648170480	2.217466968180	1.045697835815
C	-3.324257662352	-2.248725894309	2.116558033224
C	-2.481963318959	-2.987715121266	1.291413979027
C	-1.151398049113	-2.613303977640	1.143294223706
C	-3.879969991734	0.230433812315	-0.652485509625
C	-5.133275334530	0.188591224348	-1.248772176958
C	-5.256358332032	0.092687841673	-2.632349477360
C	-4.111538913821	0.040872004797	-3.420804486040
C	-2.849881645198	0.090564144102	-2.838446762501
C	0.318485814974	3.161369263100	1.895980870144
C	1.067394251366	4.240105806235	2.339319968121
C	2.409012913344	4.394594208925	1.960398052466
C	2.980340293207	3.433745250663	1.110390284270
C	2.235357493224	2.359763107305	0.657135546999
C	3.825731050935	6.429764165580	2.824183189871
O	5.824385884467	-3.843435394792	-2.748376801843
O	4.373993158304	-4.628461557304	-4.164069524308
H	0.350826782288	-2.394870082272	-2.912724953692
H	2.133850400716	-3.801529368242	-3.949494745488
H	4.999744232920	-2.226883004062	-1.183925957232
H	3.232322918546	-0.802654833050	-0.154283677571
H	1.340973831103	-1.948837644204	1.209844207410
H	2.551653267068	-0.295175261083	2.536678128830
H	1.452356701151	-1.208884251194	3.599826262330
H	1.055674441436	0.445484995922	3.109272954221
H	-1.126859227683	0.110737456677	3.170456189305
H	-3.479973140678	-0.557964164537	3.439564584132
H	-4.364297679720	-2.539052727519	2.233628252414
H	-2.860967461718	-3.858352202274	0.764536660245
H	-0.494652754139	-3.195610180751	0.499972360868
H	-3.779606075158	0.290130372546	0.424802079125
H	-6.020456408949	0.223526246089	-0.623436956767
H	-6.239086808951	0.057204352968	-3.092576897207

H	-4.195879885172	-0.031690178509	-4.501101663776
H	-1.954152197738	0.052201662166	-3.447798875775
H	-0.715163572179	3.051762781490	2.196600583128
H	0.615728205591	4.973432156209	2.999308062421
H	4.014059403917	3.546852409990	0.800430266691
H	2.683510488323	1.627527953936	-0.005123215536
H	4.398580523807	7.254841172781	3.172589537567

AlkVZ 7

C	0.922196510680	-3.066472527533	-2.048570783418
C	1.374427561095	-4.015087406185	-2.952164695278
C	0.495082397113	-4.998364158082	-3.385972318624
C	-0.821727575506	-5.057670821887	-2.936796302259
C	-1.262270467350	-4.112287598019	-2.029664441288
C	-0.399145765807	-3.099469585870	-1.578971935378
C	-0.869801793415	-2.106318812309	-0.609932088862
N	0.970928477791	-6.010007823845	-4.344681331583
N	0.096604560619	-1.340363448650	0.078169931046
N	-0.410918102239	-0.087413581130	0.471841363190
C	-1.727120495915	0.024210036624	0.912894086050
N	-2.508970083148	-1.097628465159	0.572109405974
N	-2.135164780410	-1.970716135902	-0.410422840385
C	-3.893124172271	-1.133029175615	0.927466394381
C	0.817672316284	-2.080003285261	1.179911887747
O	-2.184882856732	1.006962342512	1.457442595017
C	2.811744130620	4.355762863649	-0.839025001524
C	-0.099864043769	-2.357379100655	2.350525897616
C	2.107288892611	-1.353566672057	1.531390267908
C	-0.861298851739	-3.529310204454	2.358611499469
C	-1.773157331084	-3.777883951330	3.377915511655
C	0.379410958362	1.051686660769	0.143633497528
C	-1.930379528256	-2.857195188850	4.409561552060
C	-1.170818023676	-1.691420868540	4.416005523924
C	-0.261093427030	-1.441659261574	3.393317754436
C	-4.848579299696	-1.469624379250	-0.028501457089
C	-6.187479080046	-1.537014110733	0.339996451328
C	-6.574686983335	-1.266070906996	1.648278464247
C	-5.609459079716	-0.930600506410	2.594115144730
C	-4.267586492791	-0.867586172036	2.242894422986
C	0.414041263416	2.167704350952	0.984283941045
C	1.207811855634	3.253546196641	0.652476258469
C	1.995283922763	3.251195168863	-0.511090565184
C	1.952184383867	2.115996220809	-1.340832512357
C	1.154750444060	1.033341028294	-1.019205246762
C	3.513443864963	5.304922071054	-1.124072294693
O	2.137948205762	-5.938074838447	-4.712734693922
O	0.170127327582	-6.861045007836	-4.714103423023
C	4.329782314068	6.410746206553	-1.455297685961
C	4.368880371860	7.544496109096	-0.623601780792
C	5.171821545962	8.626294148685	-0.953375920598
C	5.947328167247	8.601534201368	-2.110490237234
C	5.915074872970	7.483120001380	-2.940657622840
C	5.116034354579	6.395244891112	-2.621561930474
H	1.592276666575	-2.284538294617	-1.706631571703
H	2.390778618344	-4.000504766385	-3.327184341822
H	-1.474479465632	-5.844611324633	-3.295389688890
H	-2.279262353306	-4.143435840944	-1.654214030070
H	1.072147085427	-3.042332208188	0.717036784338
H	1.923869356282	-0.344883505007	1.909751618358
H	2.745544599048	-1.263838266141	0.647682548994
H	2.642793441727	-1.914148157795	2.303143723035
H	-0.740144350686	-4.252054253157	1.554033848133
H	-2.360221020441	-4.691376591680	3.367879673746

H	-2.643012397676	-3.048593535373	5.206554577989
H	-1.287112065052	-0.970018193353	5.219860997556
H	0.320947065712	-0.524893259031	3.411269094270
H	-4.540874863863	-1.678554954999	-1.046670778455
H	-6.931870569684	-1.797027198944	-0.406797676196
H	-7.621989150768	-1.316575624330	1.930115336684
H	-5.900220318421	-0.722234411642	3.619477964206
H	-3.512761757840	-0.619025982242	2.979442383511
H	-0.185566719396	2.184035971283	1.884948228604
H	1.232947355301	4.119720427579	1.305652470573
H	2.545574055961	2.101166041928	-2.249297259574
H	1.126106207159	0.167251569904	-1.671055863418
H	3.762682603613	7.559548629081	0.276530276650
H	5.193117923183	9.496185826483	-0.303369689206
H	6.574140257262	9.450935533381	-2.364754453477
H	6.517422408304	7.459249779726	-3.844167777291
H	5.087444910083	5.522081075717	-3.265539163990

AlkVZ 8

C	-4.160048776758	-1.095743130145	-2.085009296503
C	-5.324271655416	-0.554344673853	-2.596561914967
C	-5.444826807865	0.830729738227	-2.678102918379
C	-4.431175351661	1.680853299531	-2.255862550217
C	-3.269908266943	1.129889276806	-1.737398131072
C	-3.120039841815	-0.261567835790	-1.641741881725
C	-1.885395197583	-0.841617745051	-1.107436366992
N	-6.679721473936	1.410154411928	-3.231676087875
N	-0.748048434832	-0.010834178968	-1.010795259018
N	0.116297220400	-0.423041644050	0.020945024737
C	0.310551207134	-1.777710881477	0.266820465798
N	-0.669599222423	-2.585779794001	-0.345997864201
N	-1.872908265577	-2.079997918525	-0.751987714279
C	-0.629880568901	-4.003281882204	-0.169577914966
C	-0.049739137942	0.259809423084	-2.320377964067
O	1.173977378100	-2.224624740006	0.993270467560
C	0.623879359396	-0.985132819673	-2.855456664265
C	0.859102544618	1.471675597891	-2.180466741376
C	1.930630572907	-1.328068047081	-2.498150154665
C	2.494319105524	-2.519164385570	-2.944808118527
C	0.528286662800	0.582092870853	0.946326219570
C	1.760179283185	-3.383226627650	-3.751446937157
C	0.460028536010	-3.048128288542	-4.117185572409
C	-0.100435604707	-1.855444309377	-3.674811234150
C	0.555139075739	-4.689267493978	-0.427132372729
C	0.588372528745	-6.069599914853	-0.281420831535
C	-0.551518538638	-6.768350456155	0.107572176331
C	-1.731385370003	-6.073479299300	0.352910430914
C	-1.777455852854	-4.690310344577	0.219184847930
C	1.804714652740	0.554569383475	1.510397297850
C	2.185063113028	1.556994477614	2.390751846393
C	1.319108678749	2.604781395174	2.720363890073
C	0.045855468068	2.622174889236	2.136804242356
C	-0.346476476510	1.623732239760	1.261747194865
O	-6.751416302838	2.631815117717	-3.303269171897
O	-7.559623184848	0.634352562613	-3.587747174180
H	-4.036089293923	-2.171323926118	-2.021692979725
H	-6.136423937467	-1.182960958147	-2.941834609352
H	-4.563922372228	2.753518164779	-2.331254184195
H	-2.471808267952	1.778616671225	-1.391627746193
H	-0.871747479886	0.517031968401	-3.001374254512
H	1.326457255972	1.688677960737	-3.145434019765
H	1.652419605338	1.311498633151	-1.446159793202
H	0.282917645842	2.343765051173	-1.858358736088
H	2.515486361687	-0.667605766937	-1.864848575534
H	3.510977399852	-2.773001047368	-2.658135301079
H	2.199925306881	-4.315014963685	-4.095087335616
H	-0.117674956005	-3.715497217983	-4.749713639628
H	-1.116655425396	-1.596270575379	-3.965211296037
H	1.435419766303	-4.142357278276	-0.743351081142
H	1.512702273992	-6.603214787626	-0.481962728243
H	-0.520303343087	-7.848143275984	0.216847561031
H	-2.625769690967	-6.608302813690	0.658744950017
H	-2.693185978510	-4.142570379886	0.409948203585

H	2.486585837240	-0.248782898140	1.263517061996
H	3.186804136763	1.527872900450	2.810593716492
H	-0.638480273196	3.425115166241	2.389716815552
H	-1.338583165798	1.642996757402	0.824062005719
C	1.716883534815	3.659225981963	3.646018884088
N	0.977674824121	4.801541346009	3.809037145253
N	1.547275709859	5.563648610221	4.694201172335
N	2.657968754174	4.928809523789	5.122762833275
C	2.806875912882	3.740890812573	4.492063961688
H	3.639306416879	3.083947800410	4.693671858076
C	3.540783103269	5.551948108848	6.102620220114
H	3.043002528126	6.483203436636	6.395029662299
H	3.607389155286	4.909015747596	6.988351290879
C	4.916261551202	5.820309939882	5.539308624643
C	6.054854618188	5.402128755724	6.224293807956
C	5.055360217543	6.502619589922	4.328753223786
C	7.322376554361	5.668790272237	5.711810039576
C	6.319269394862	6.763943137057	3.815503018116
C	7.456164742235	6.349023955576	4.506855528925
H	5.952211627613	4.864784552101	7.164361001796
H	4.167353284287	6.822495429981	3.788417490575
H	8.204196805435	5.338980479226	6.253221222921
H	6.419312642822	7.294769086814	2.873338952804
H	8.443536230430	6.554316439983	4.103963394875

Section S5. NMR Spectra

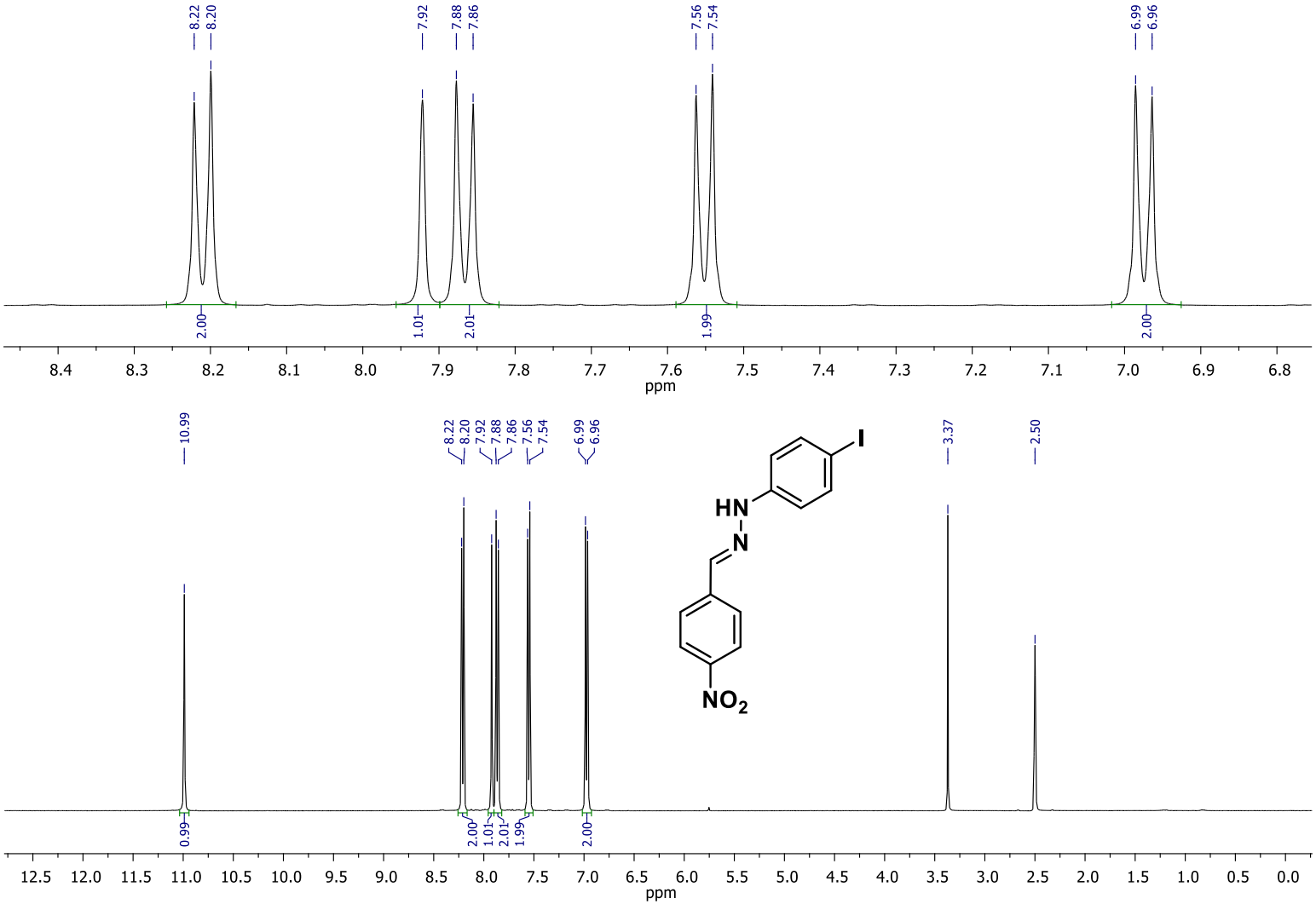


Figure S5.1. ^{1}H NMR spectrum (DMSO-d_6) of 1-(4-iodophenyl)-2-(4-nitrobenzylidene)hydrazine **9**

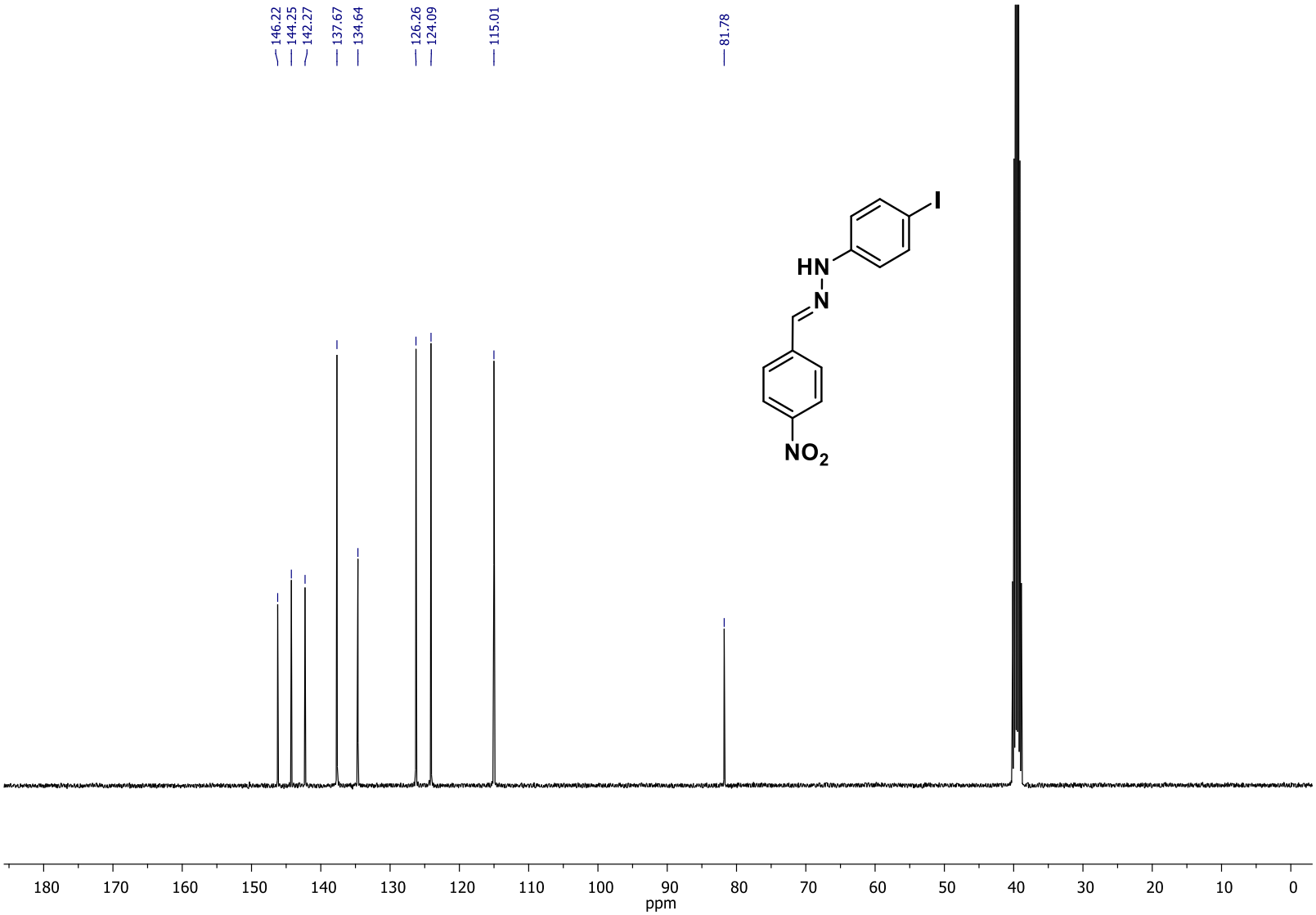


Figure S5.2. $^{13}C\{^{1}H\}$ NMR spectrum (DMSO-d_6) of 1-(4-iodophenyl)-2-(4-nitrobenzylidene)hydrazine **9**

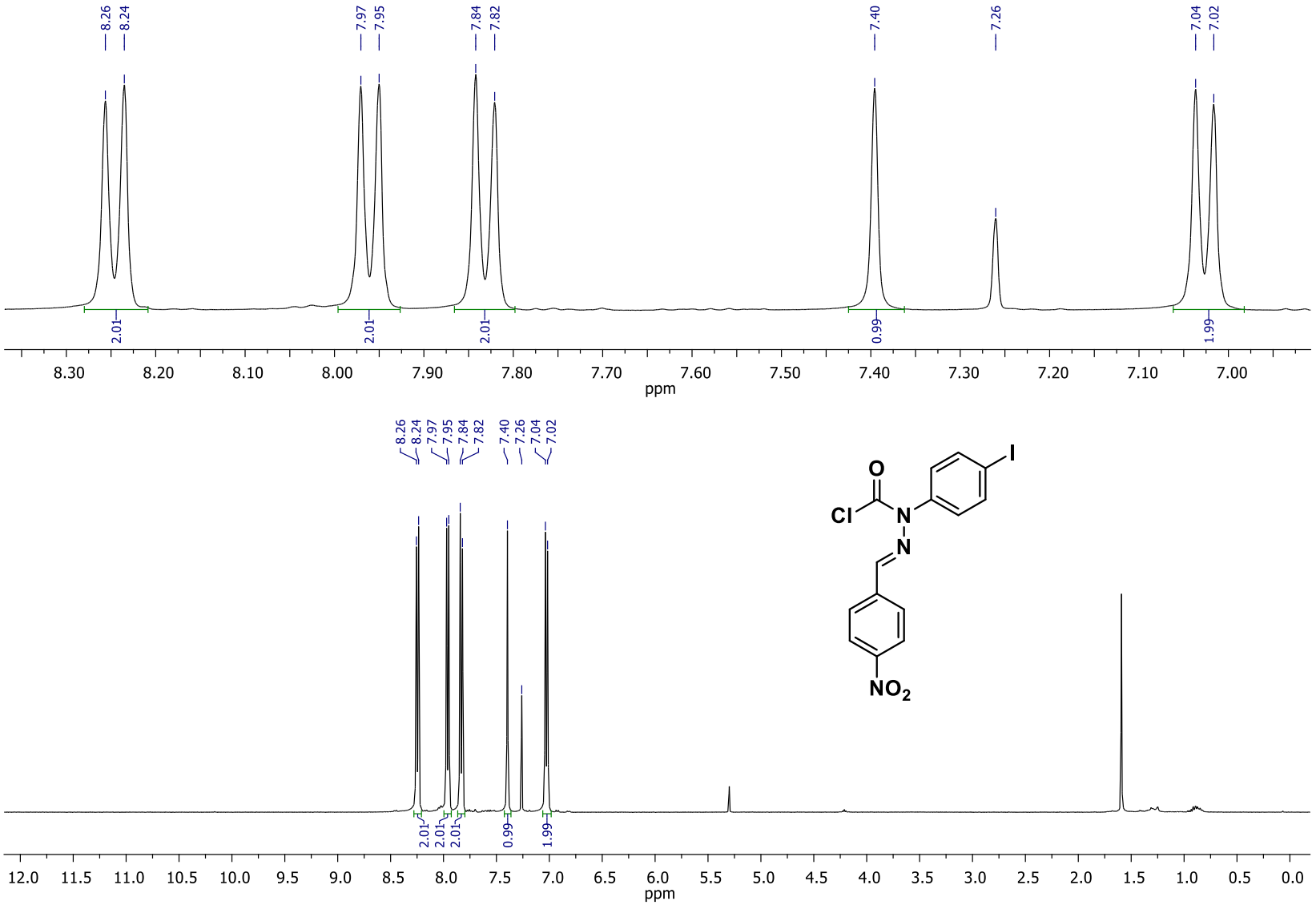


Figure S5.3. ^{1}H NMR spectrum ($CDCl_3$) of 1-(4-iodophenyl)-2-(4-nitrobenzylidene)hydrazine-1-carbonyl chloride **10**

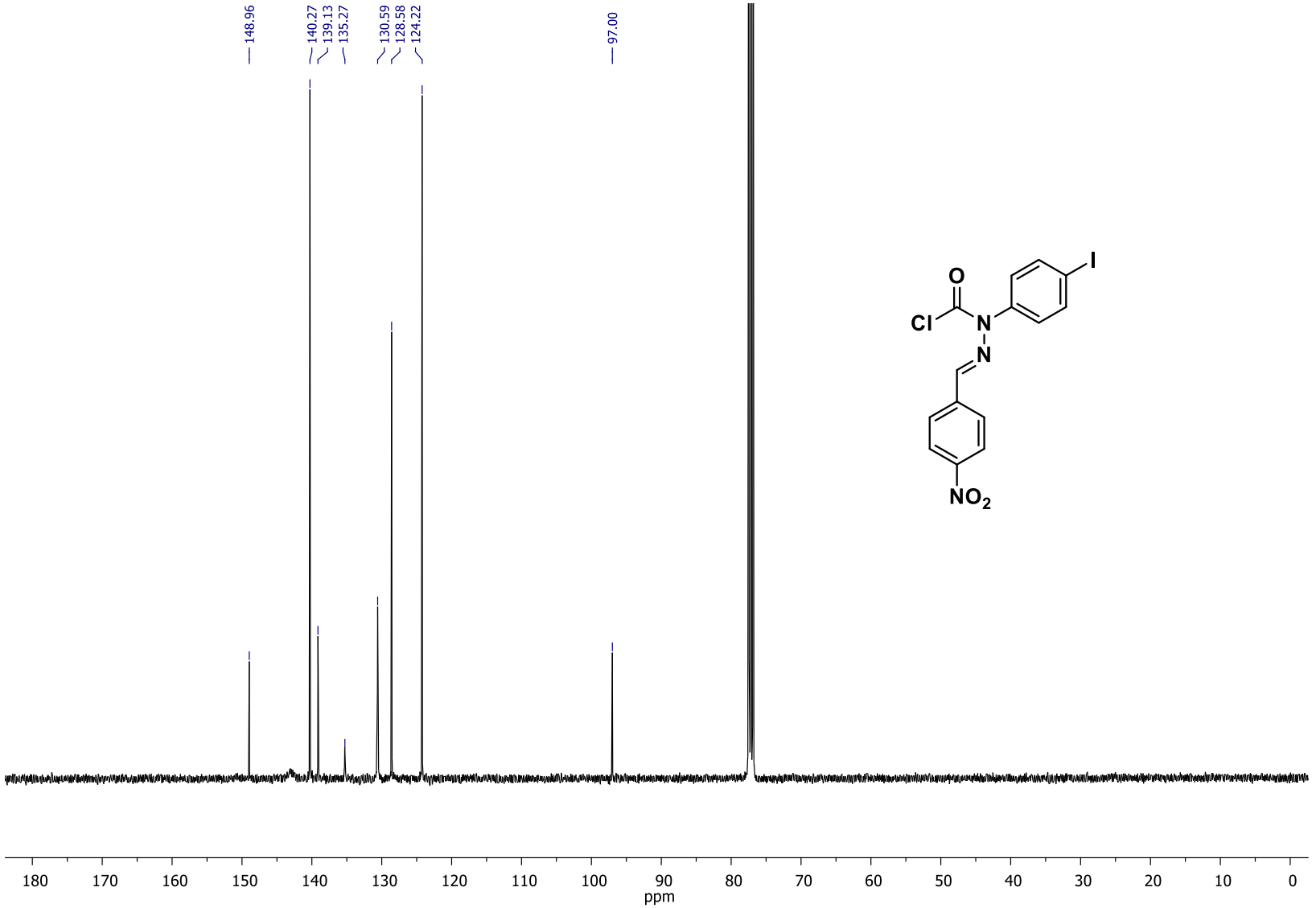


Figure S5.4. $^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$) of 1-(4-iodophenyl)-2-(4-nitrobenzylidene)hydrazine-1-carbonyl chloride **10**

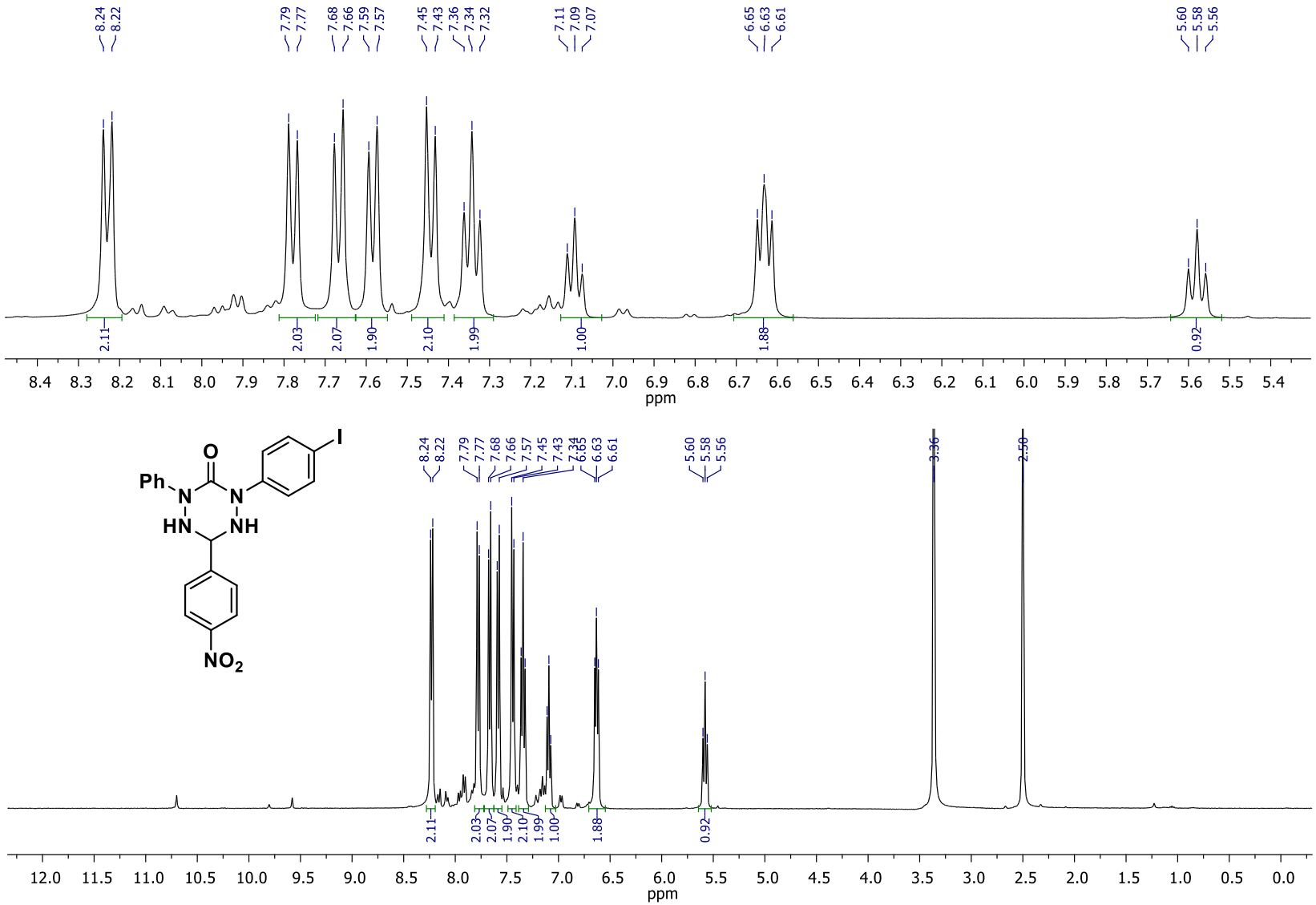


Figure S5.5. ^{1}H NMR spectrum (DMSO-d_6) of 2-(4-iodophenyl)-6-(4-nitrophenyl)-4-phenyl-1,2,4,5-tetrazinan-3-one **11**

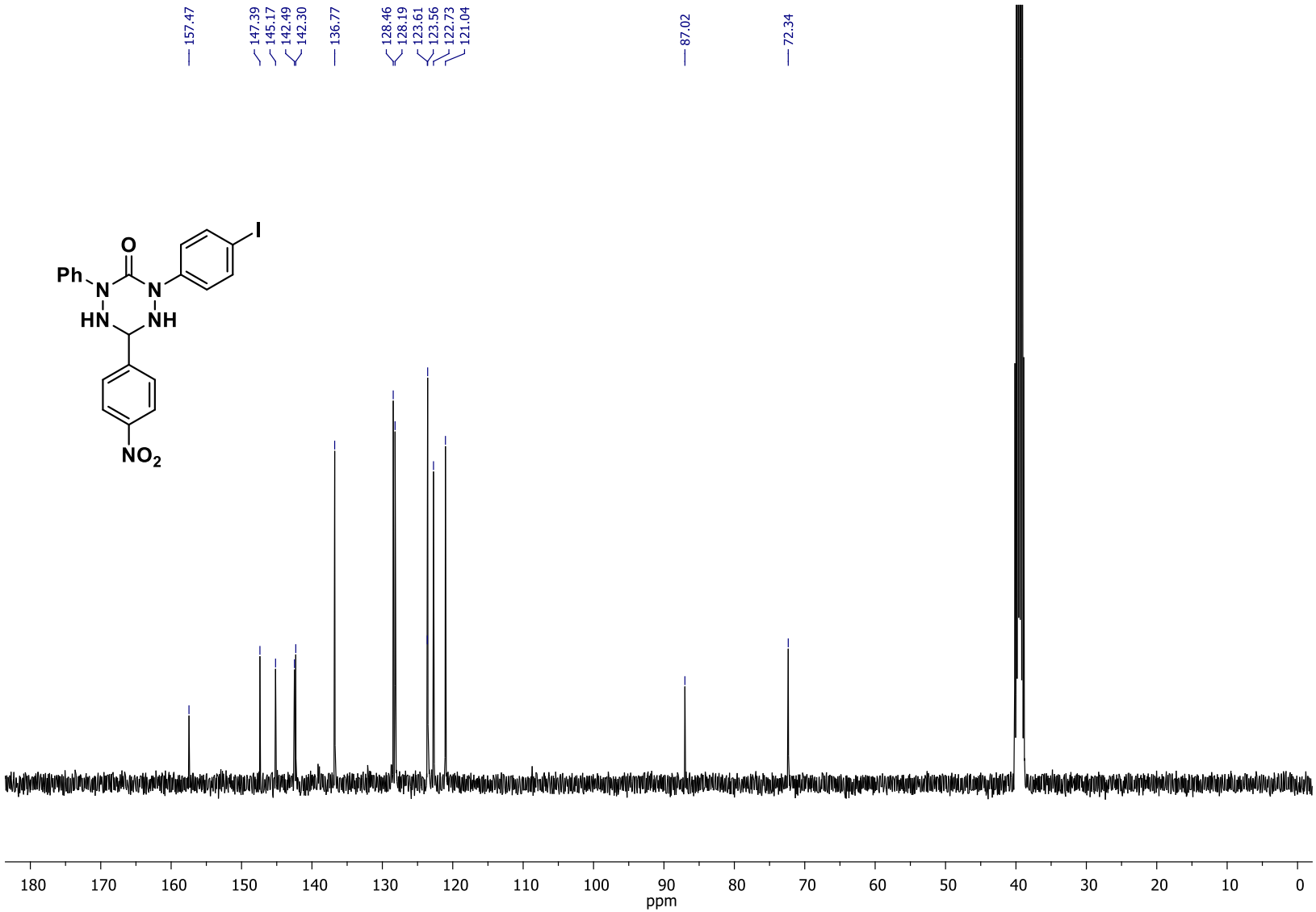


Figure S5.6. $^{13}C\{^{1}H\}$ spectrum (DMSO-d_6) of 2-(4-iodophenyl)-6-(4-nitrophenyl)-4-phenyl-1,2,4,5-tetrazinan-3-one **11**

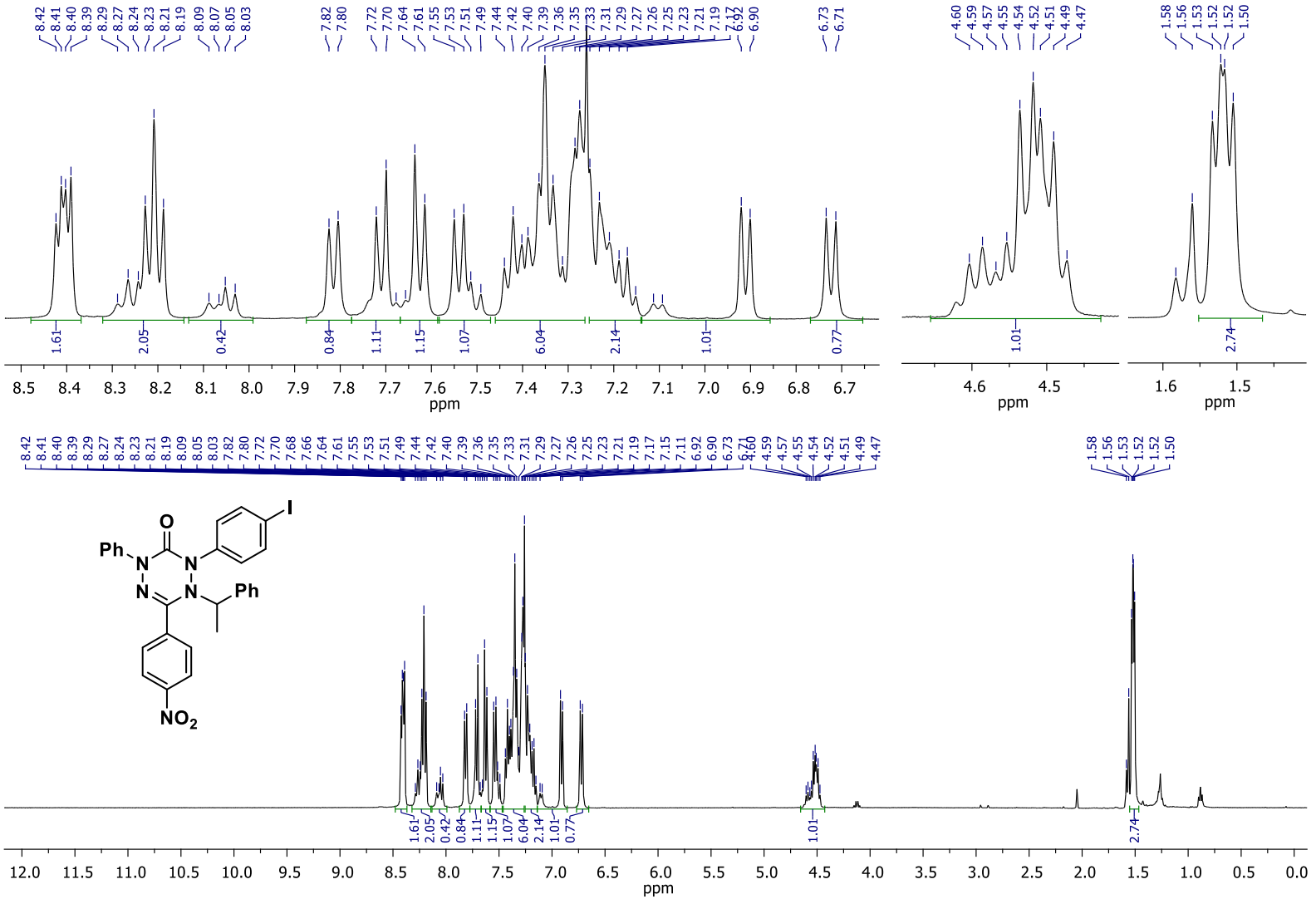


Figure S5.7. ^{1}H NMR spectrum ($CDCl_3$) of 2-(4-iodophenyl)-6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **13**

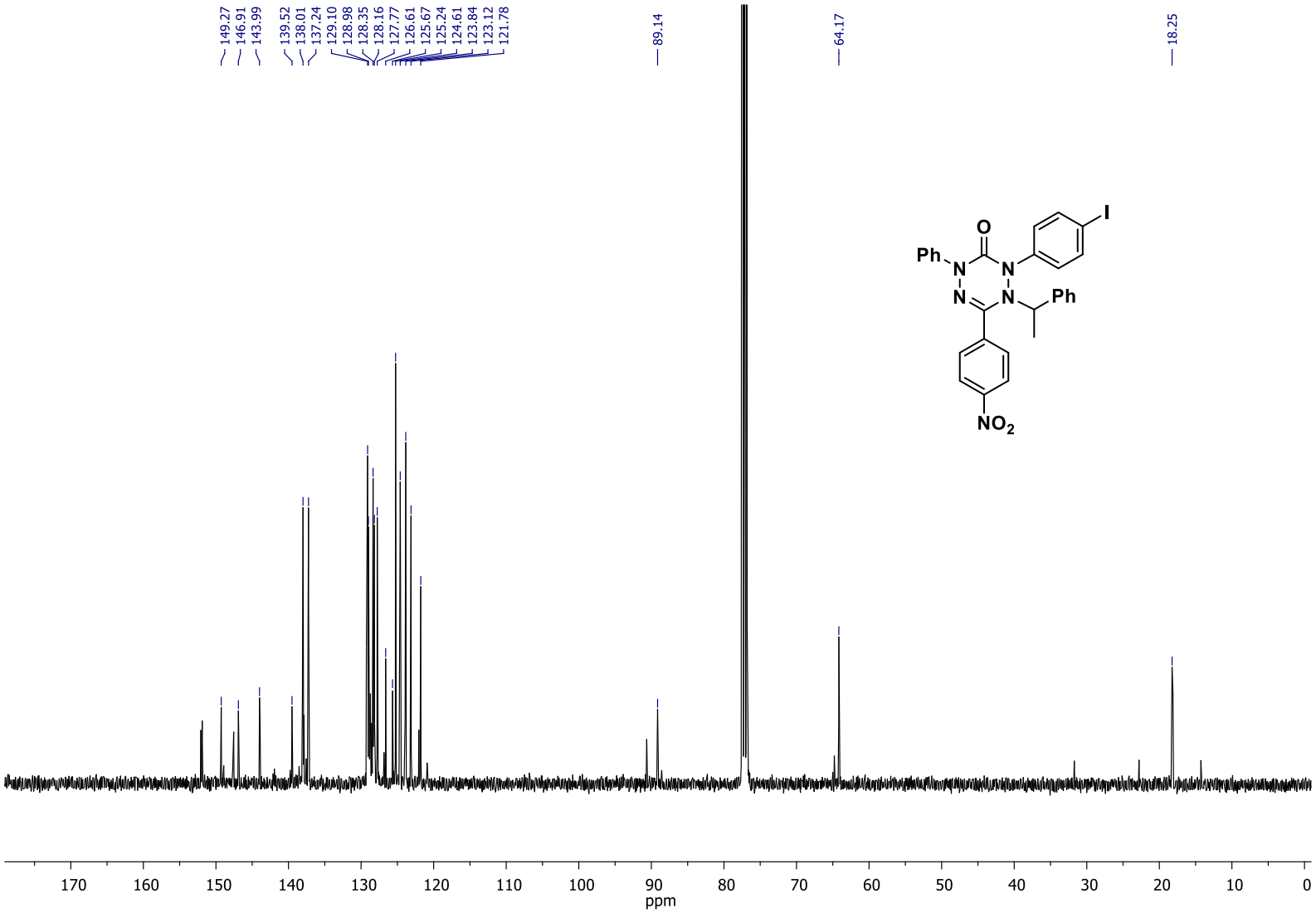


Figure S5.8. $^{13}C\{^{1}H\}$ spectrum ($CDCl_3$) of 2-(4-iodophenyl)-6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **13**

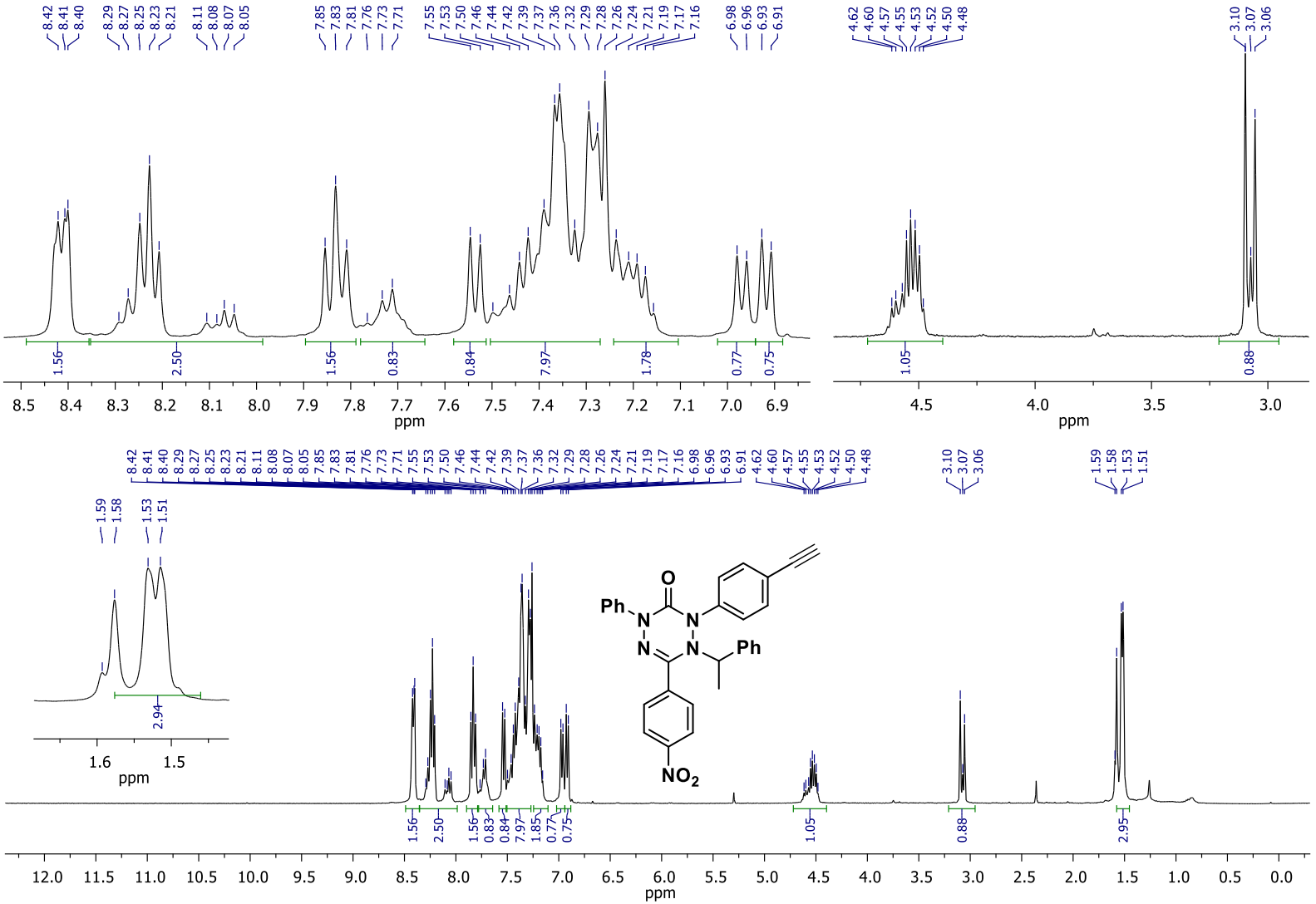


Figure S5.9. ^{1}H NMR spectrum ($CDCl_3$) of 2-(4-ethynylphenyl)-6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **6**

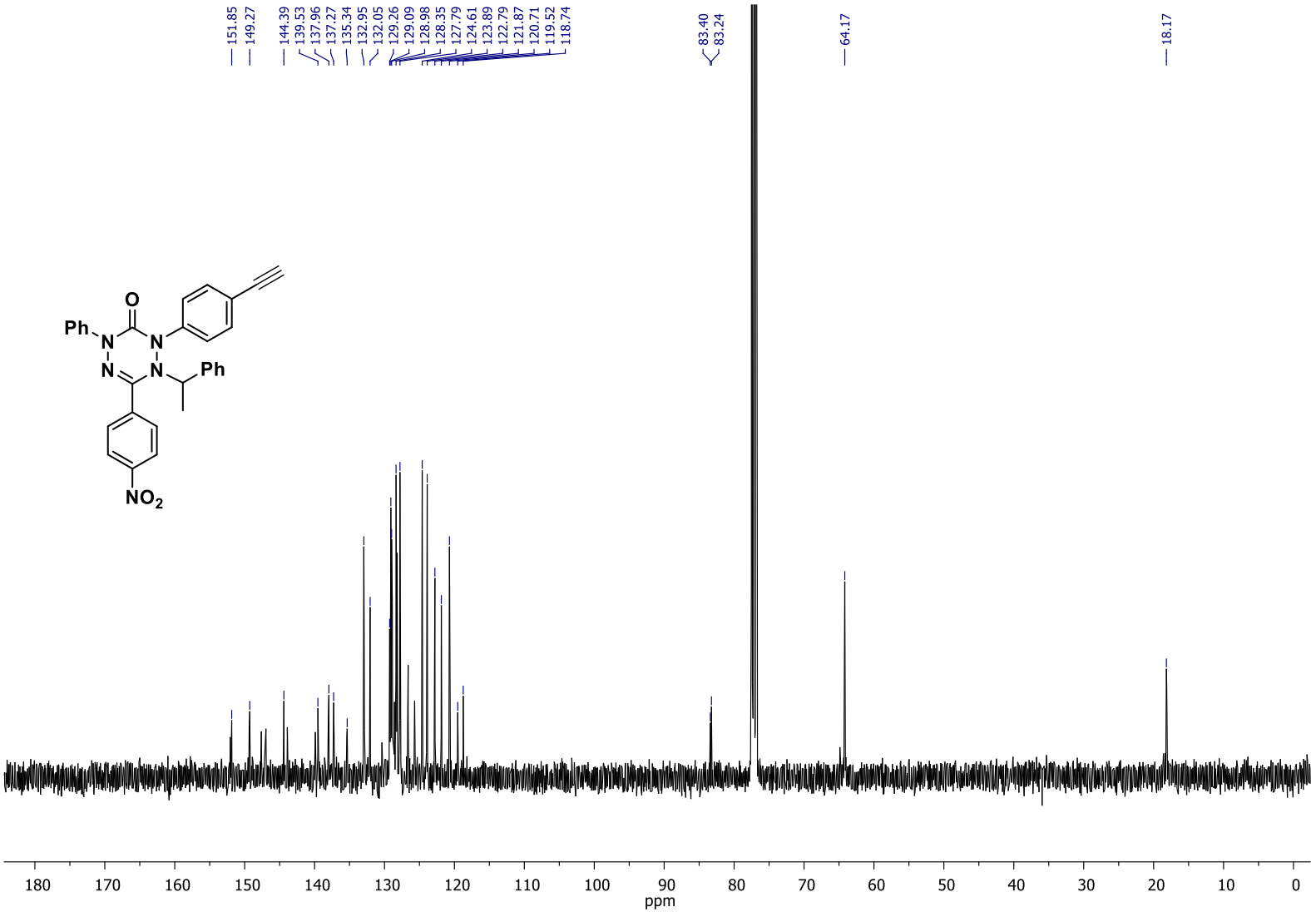


Figure S5.10. $^{13}C\{^{1}H\}$ spectrum ($CDCl_3$) of 2-(4-ethynylphenyl)-6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **6**

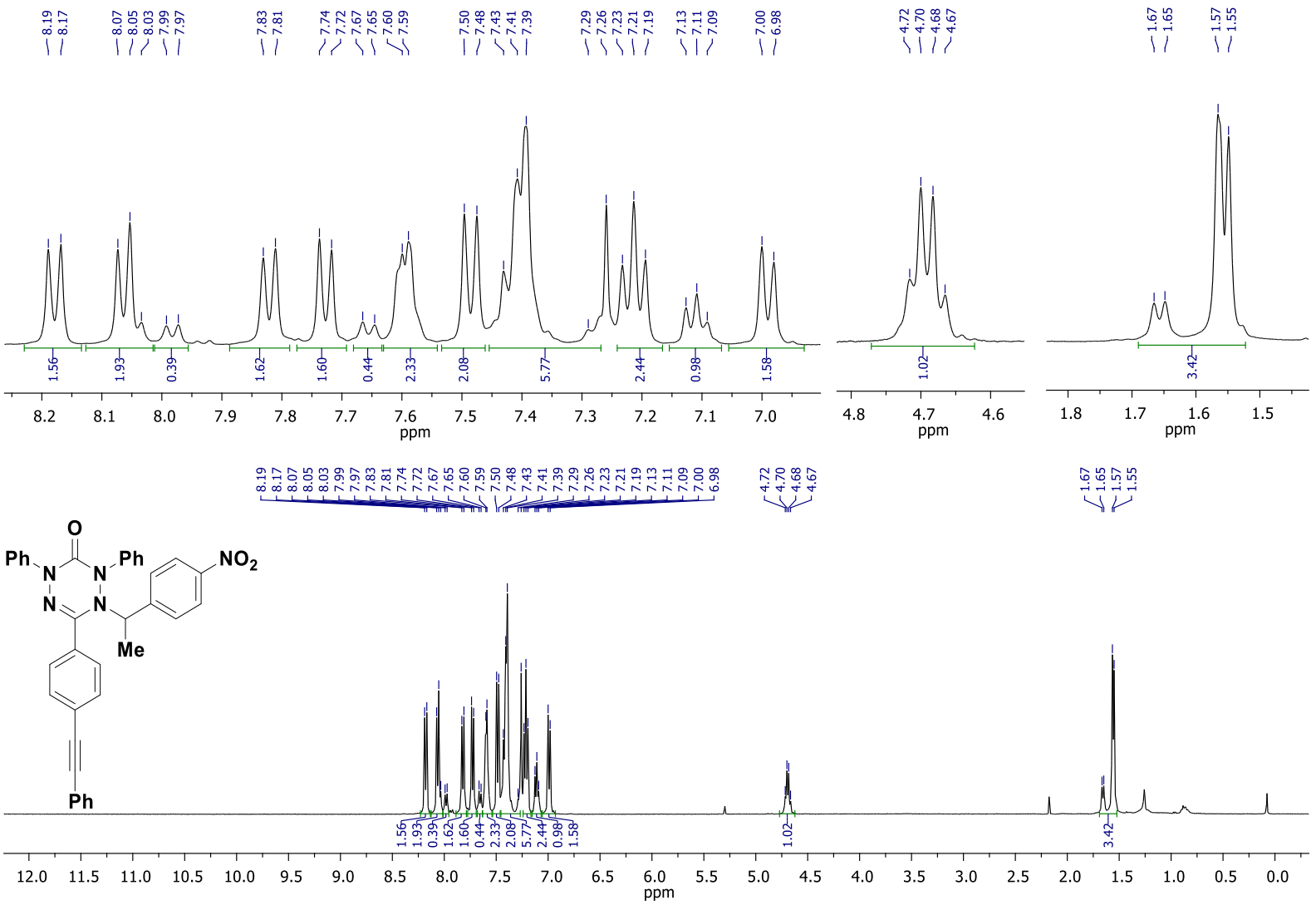


Figure S5.11. ^{1}H NMR spectrum ($CDCl_3$) of 1-(1-(4-nitrophenyl)ethyl)-2,4-diphenyl-6-(4-(phenylethynyl)phenyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **3**

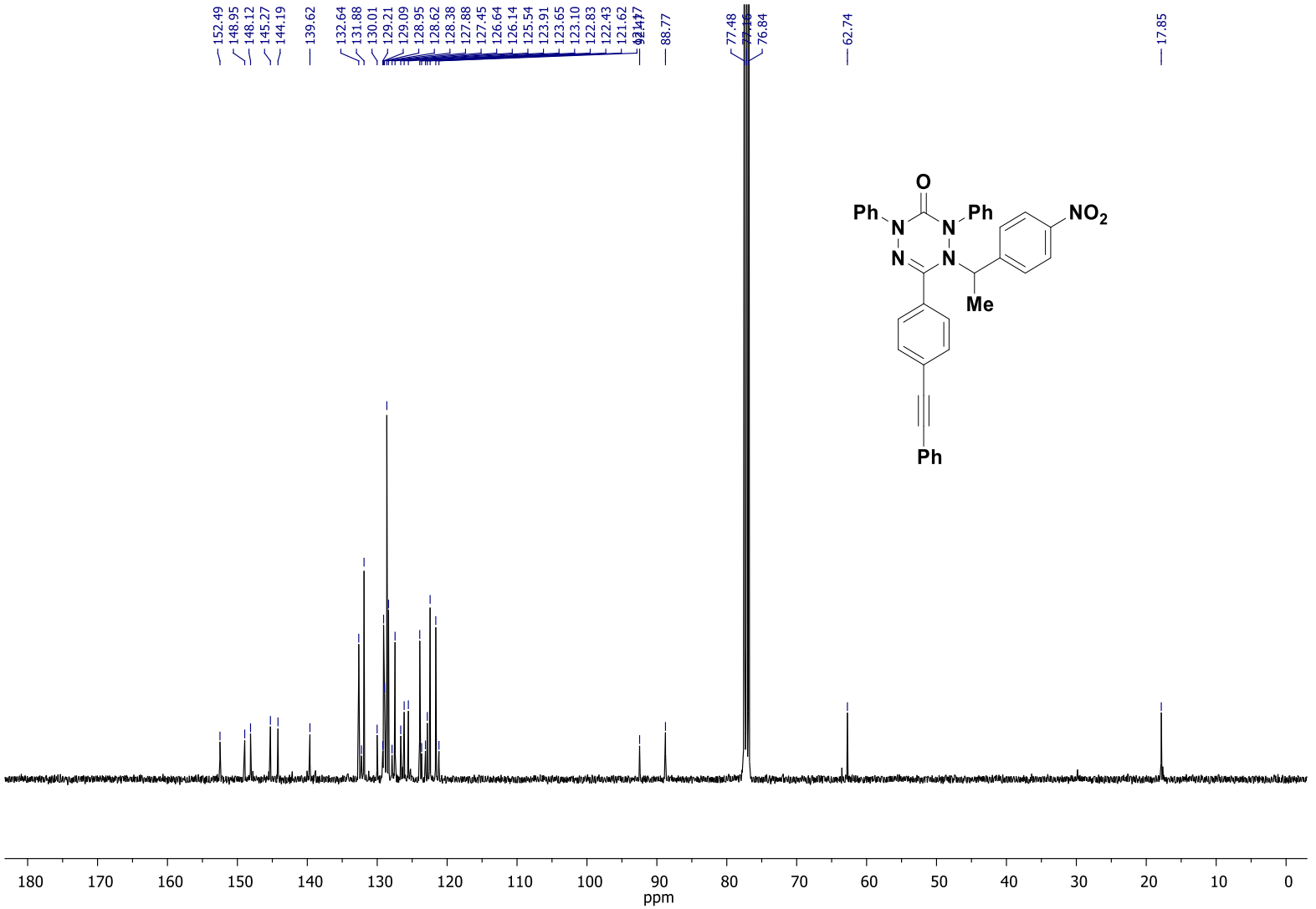


Figure S5.12. $^{13}C\{^{1}H\}$ spectrum ($CDCl_3$) of 1-(1-(4-nitrophenyl)ethyl)-2,4-diphenyl-6-(4-(phenylethynyl)phenyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **3**

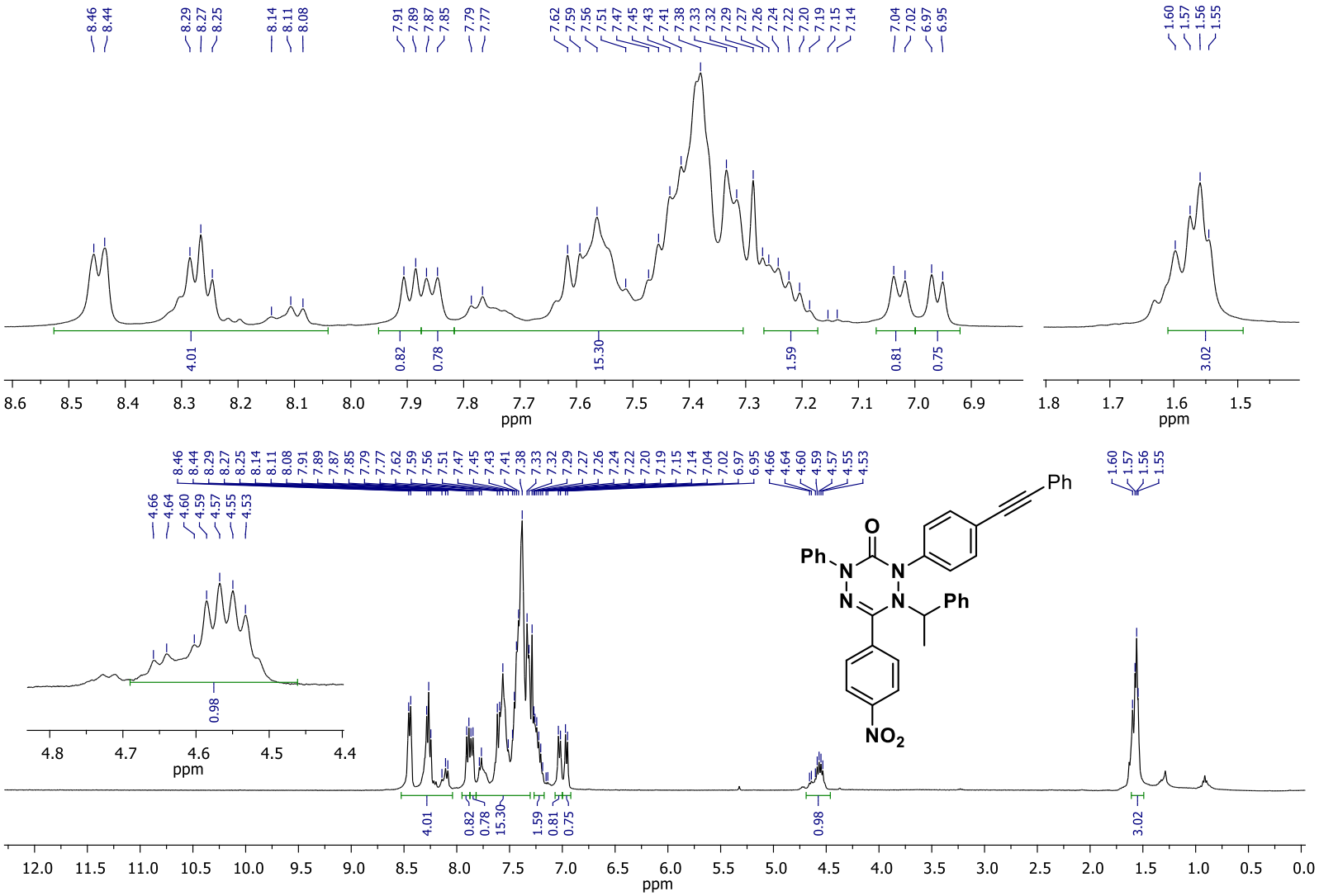


Figure S5.13. ^{1}H NMR spectrum ($CDCl_3$) of 6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-2-(4-(phenylethynyl)phenyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **7**

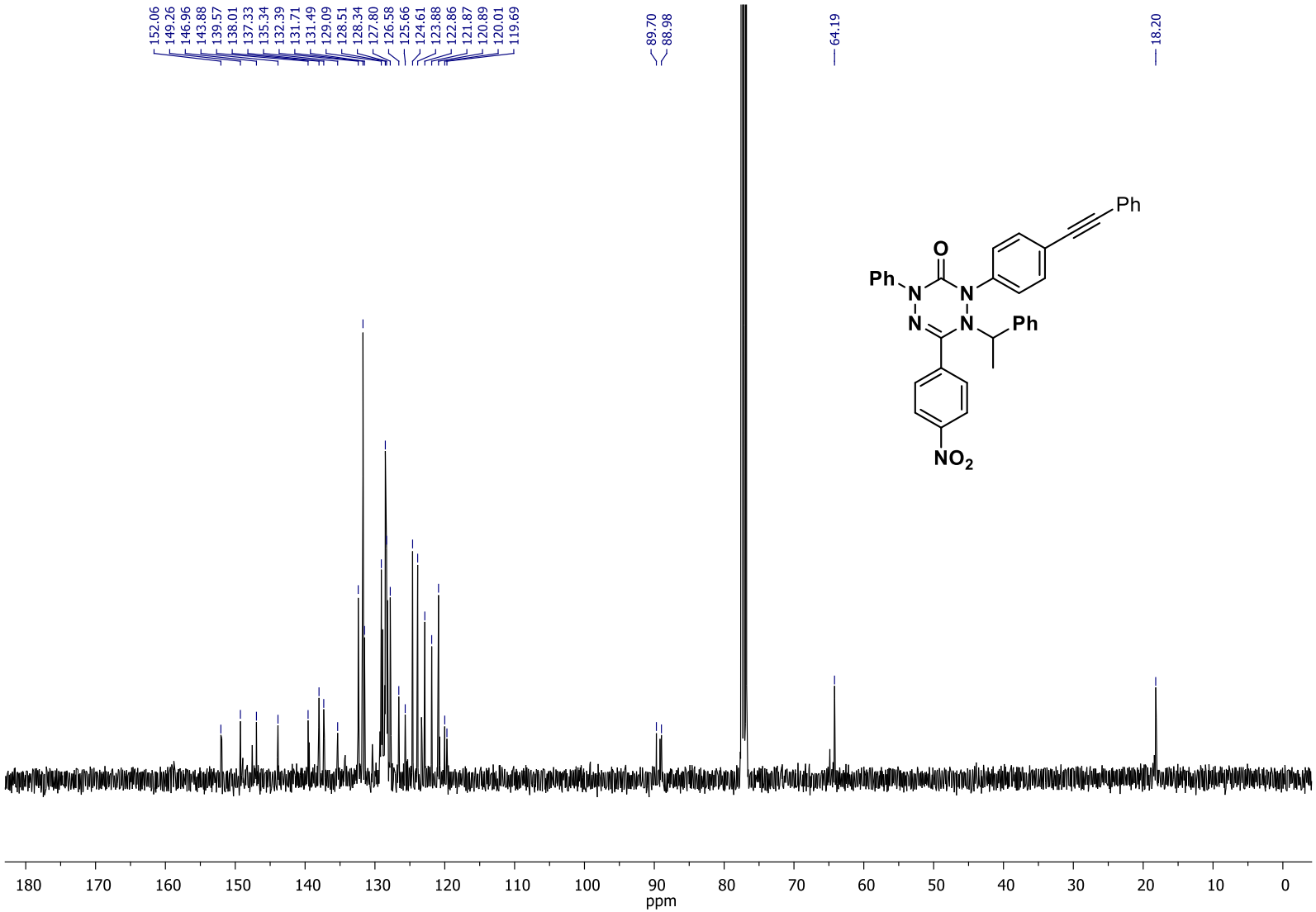


Figure S5.14. $^{13}C\{^{1}H\}$ spectrum ($CDCl_3$) of 6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-2-(4-(phenylethynyl)phenyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **7**

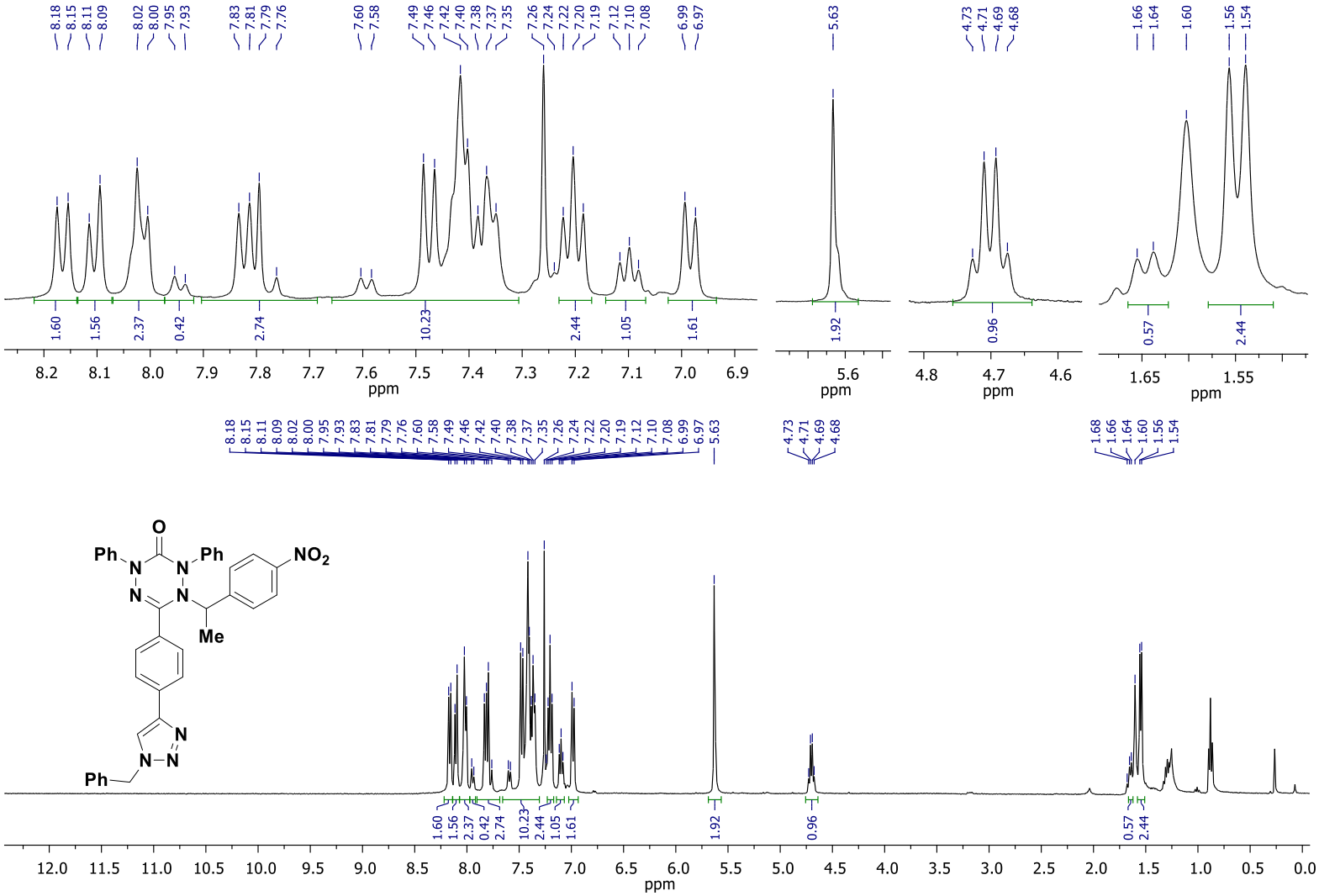


Figure S5.15. ^{1}H NMR spectrum ($CDCl_3$) of 6-(4-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)-1-(1-(4-nitrophenyl)ethyl)-2,4-diphenyl-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **4**

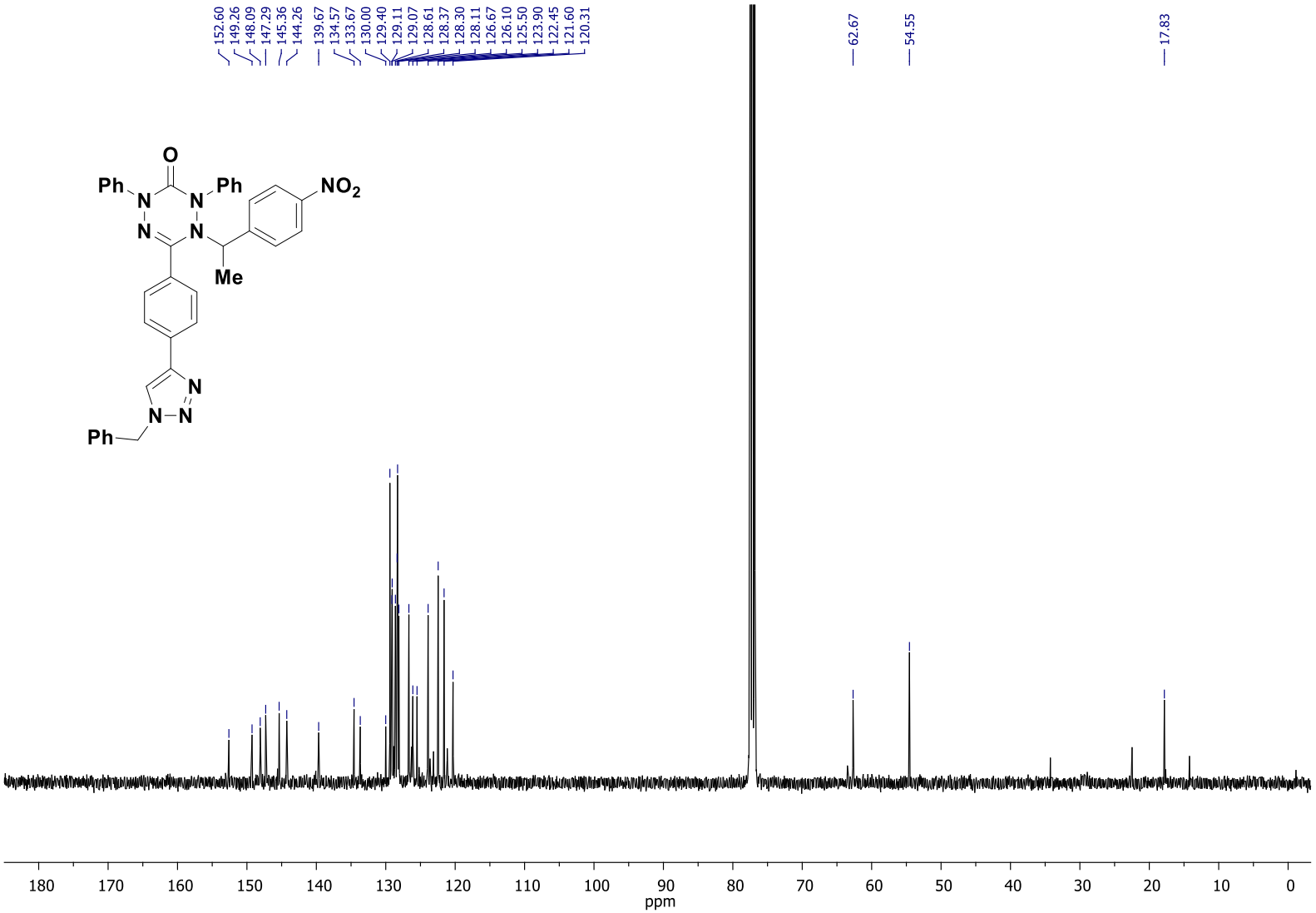


Figure S5.16. $^{13}C\{^{1}H\}$ spectrum ($CDCl_3$) of 6-(4-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)-1-(1-(4-nitrophenyl)ethyl)-2,4-diphenyl-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **4**

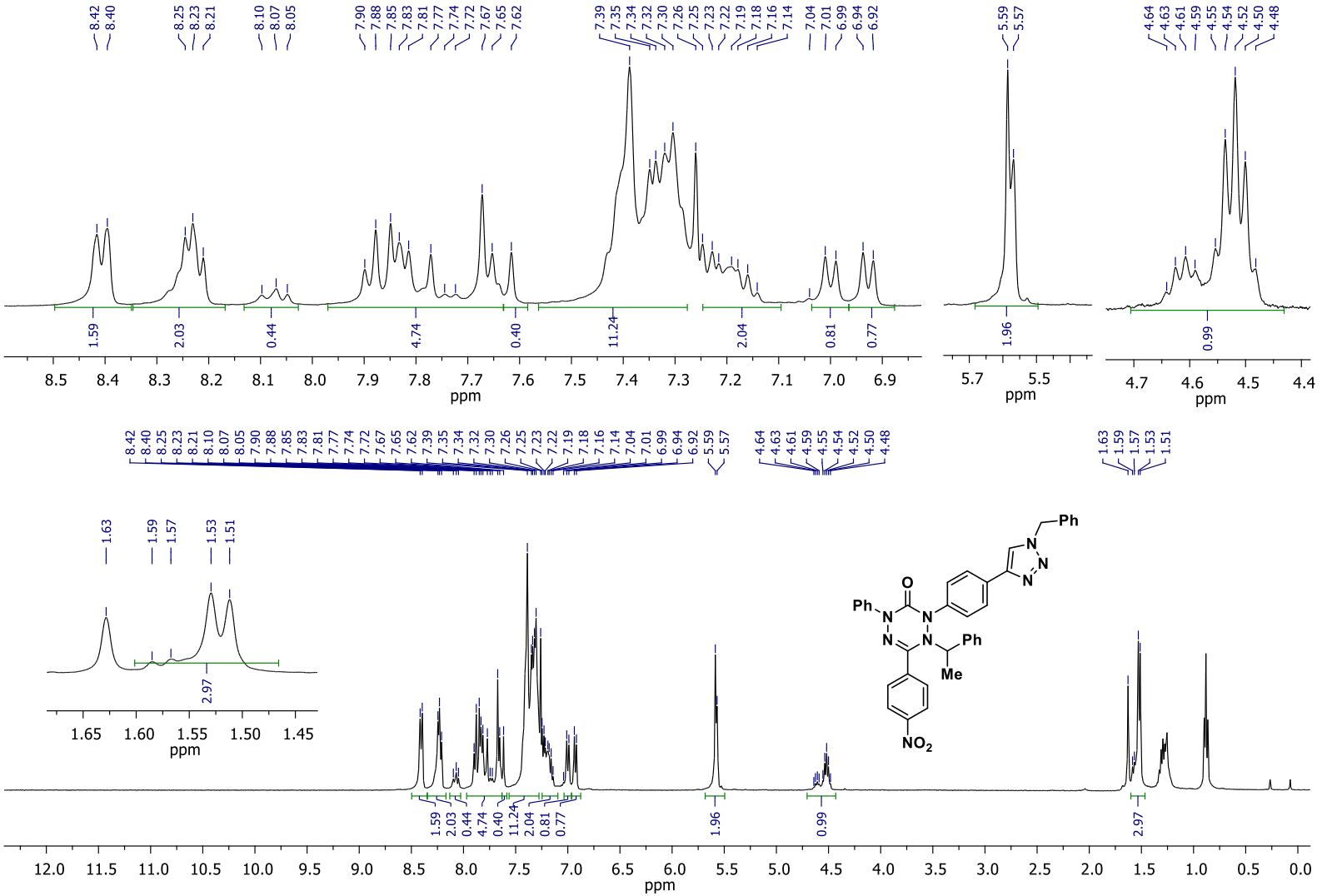


Figure S5.17. ^{1}H NMR spectrum ($CDCl_3$) of 2-(4-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)-6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **8**

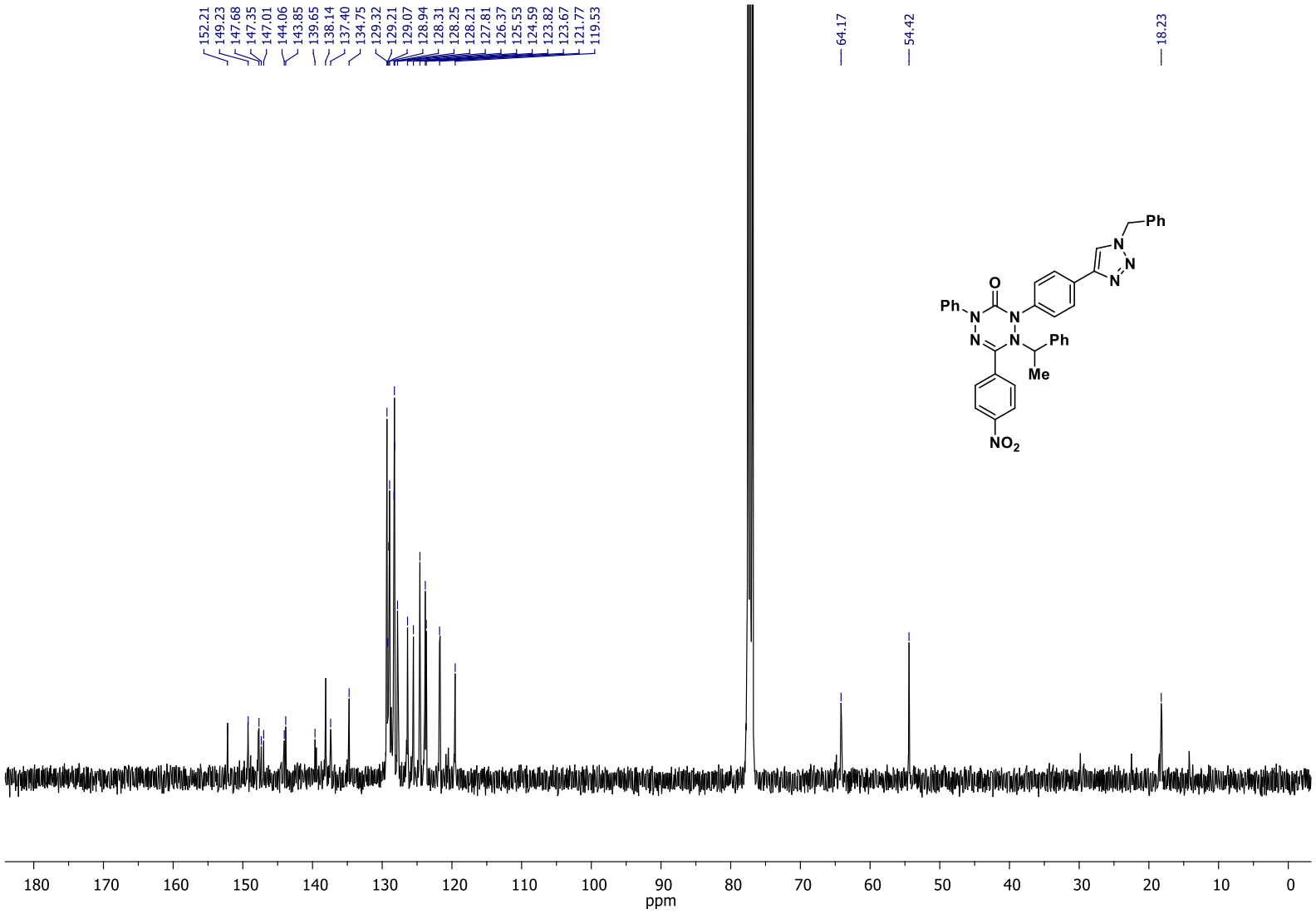


Figure S5.18. $^{13}C\{^{1}H\}$ spectrum ($CDCl_3$) of 2-(4-(1-benzyl-1H-1,2,3-triazol-4-yl)phenyl)-6-(4-nitrophenyl)-4-phenyl-1-(1-phenylethyl)-1,4-dihydro-1,2,4,5-tetrazin-3(2H)-one **8**