Electronic Supplementary Information (ESI) for New Journal of Chemistry

Bio-Activated Intramolecular *Anti*-Aza-Michael Addition: Stereoselective Synthesis of Hydantoin Derivatives

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† Deceased.

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Spectroscopic characterization of 10

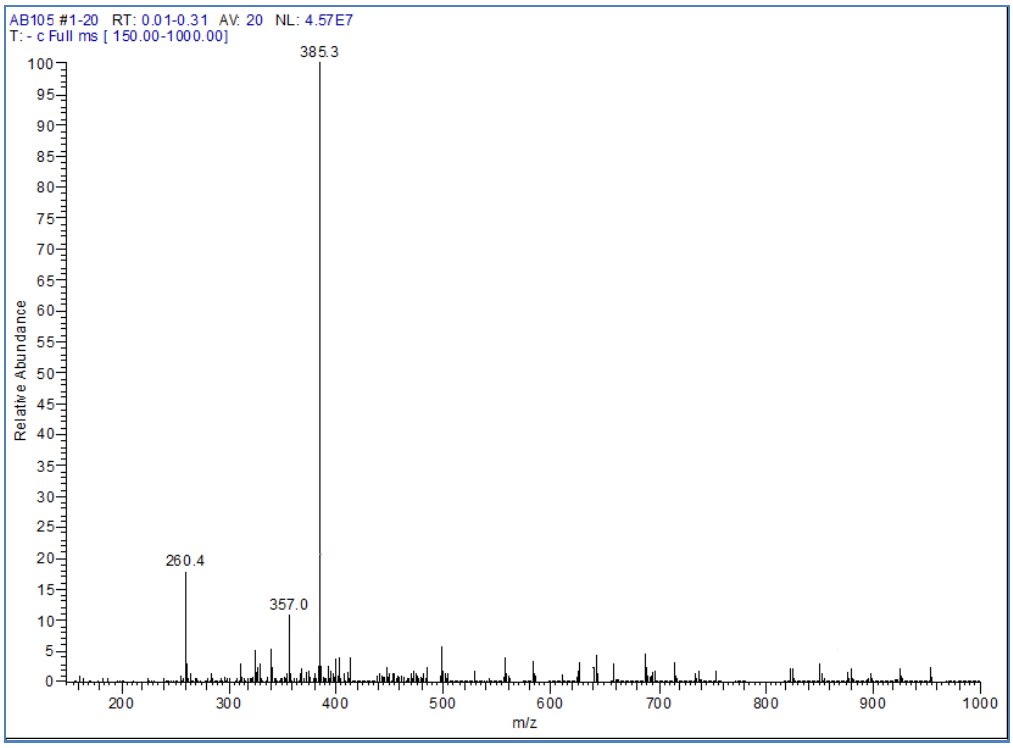

Figure S1. ESI MS spectrum of **10**.

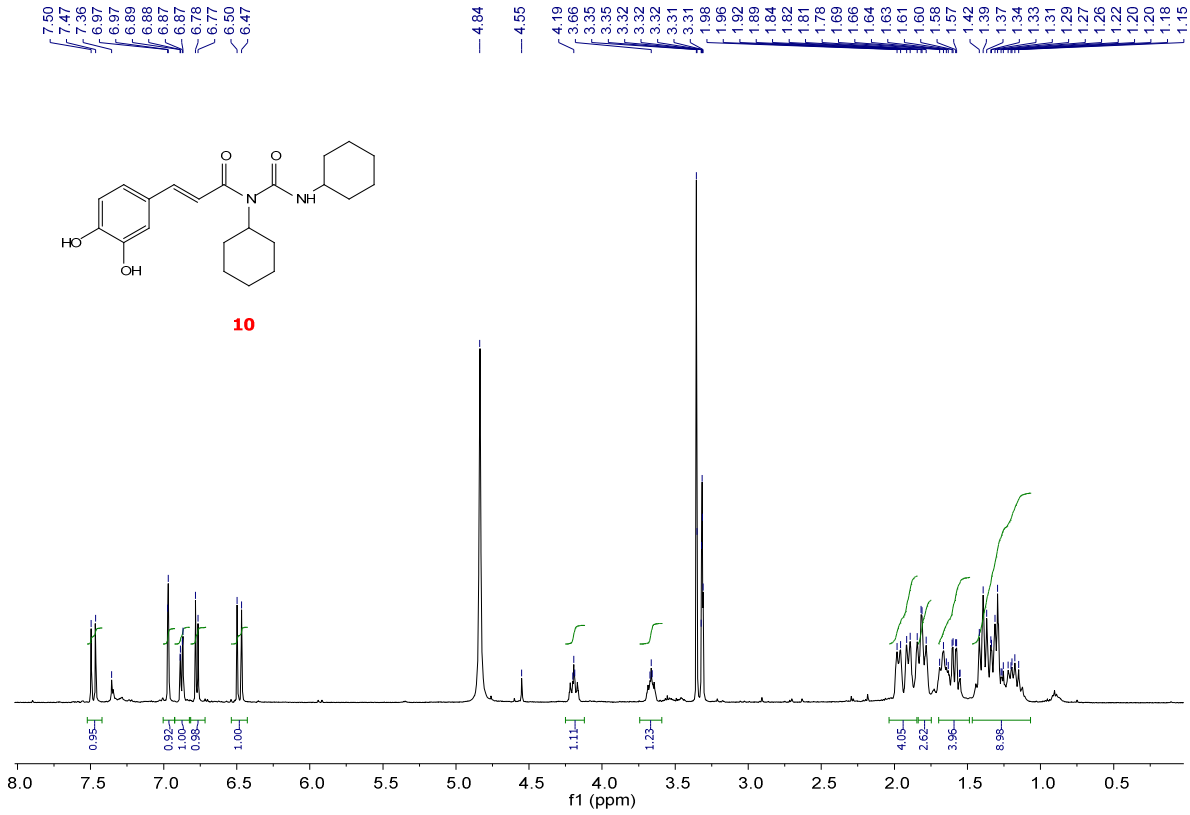

Figure S2. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **10**.

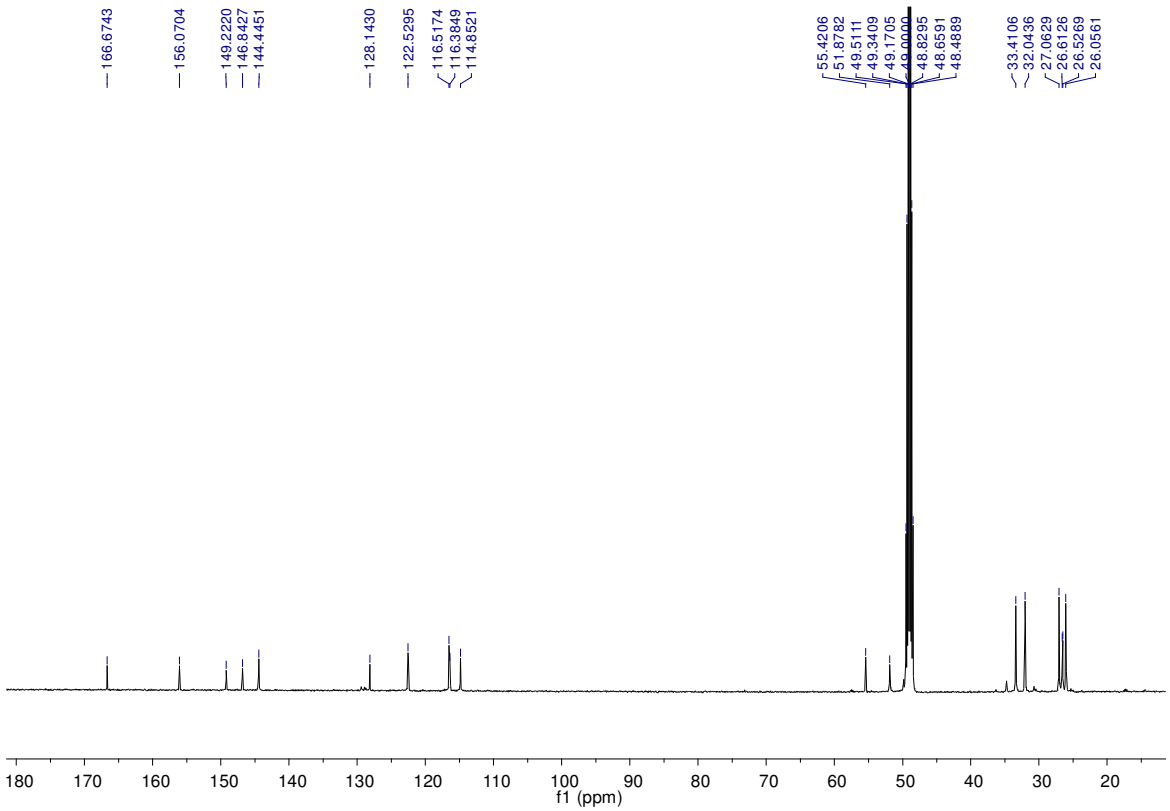

Figure S3. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **10**.

Spectroscopic characterization of 11

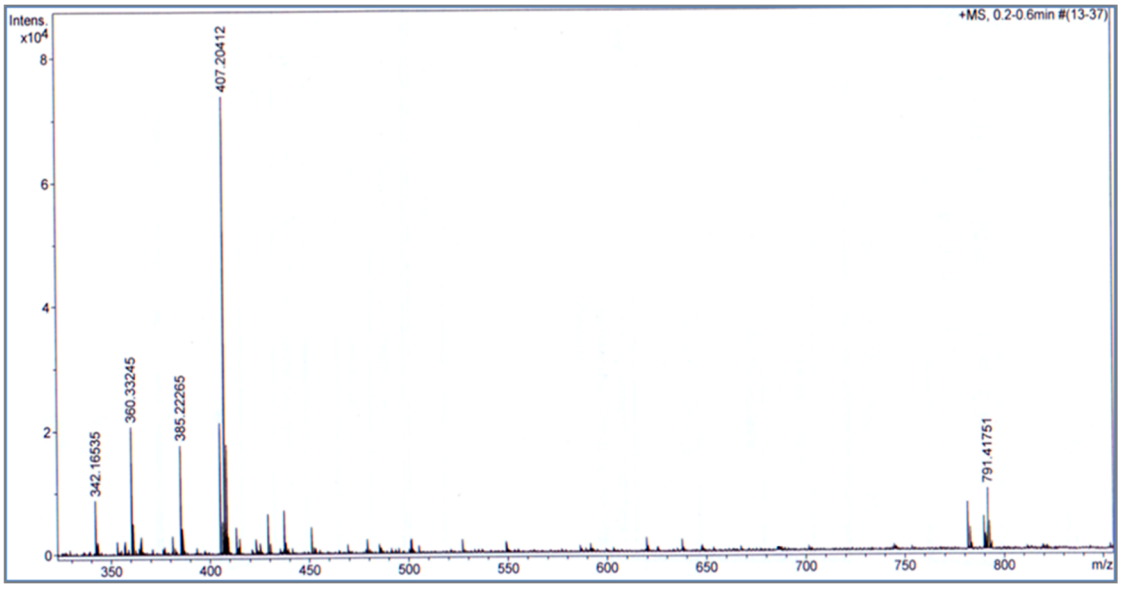

Figure S4. ESI MS spectrum of **11**.

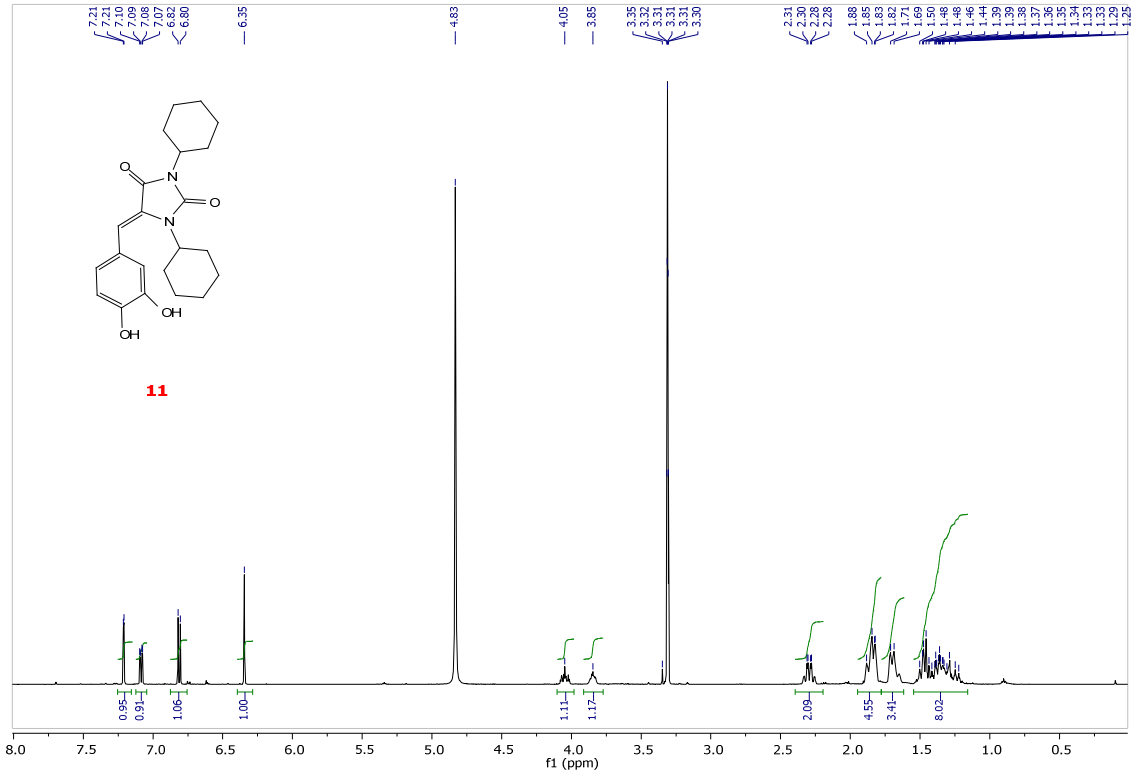

Figure S5. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **11**.

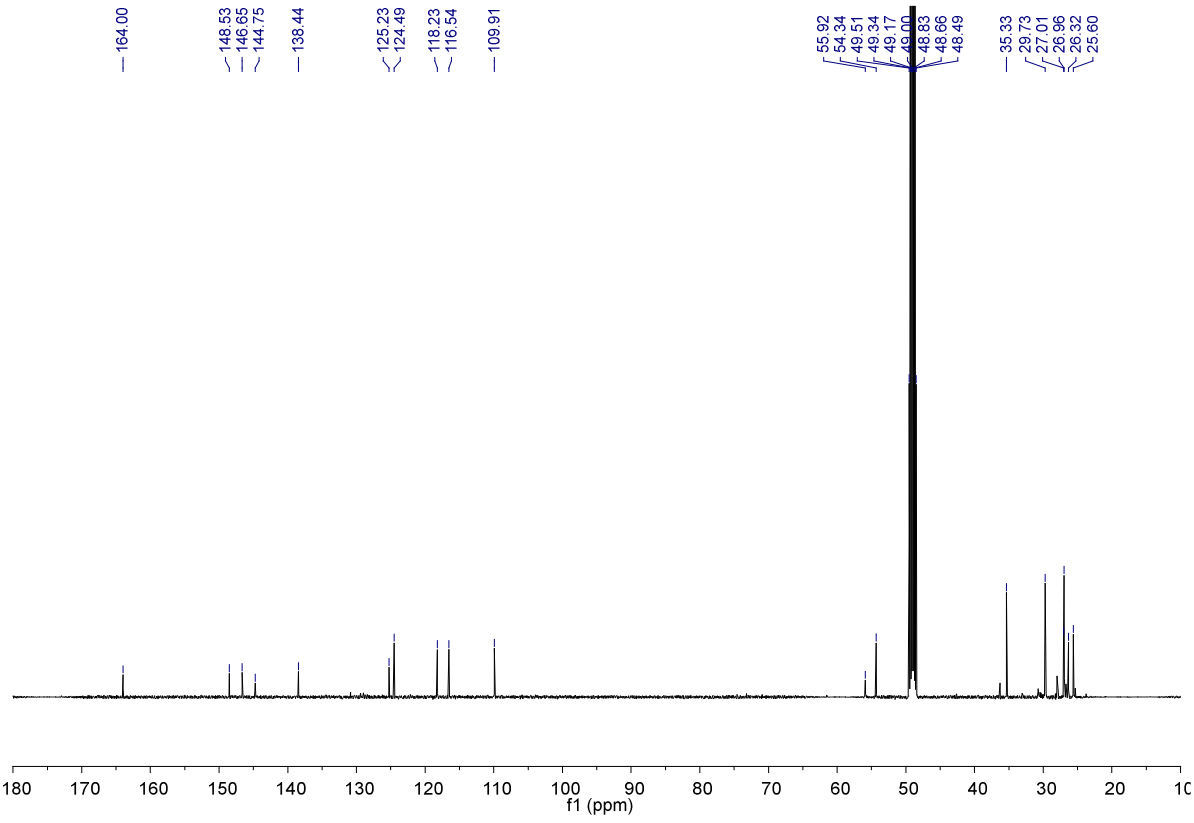

Figure S6. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **11**.

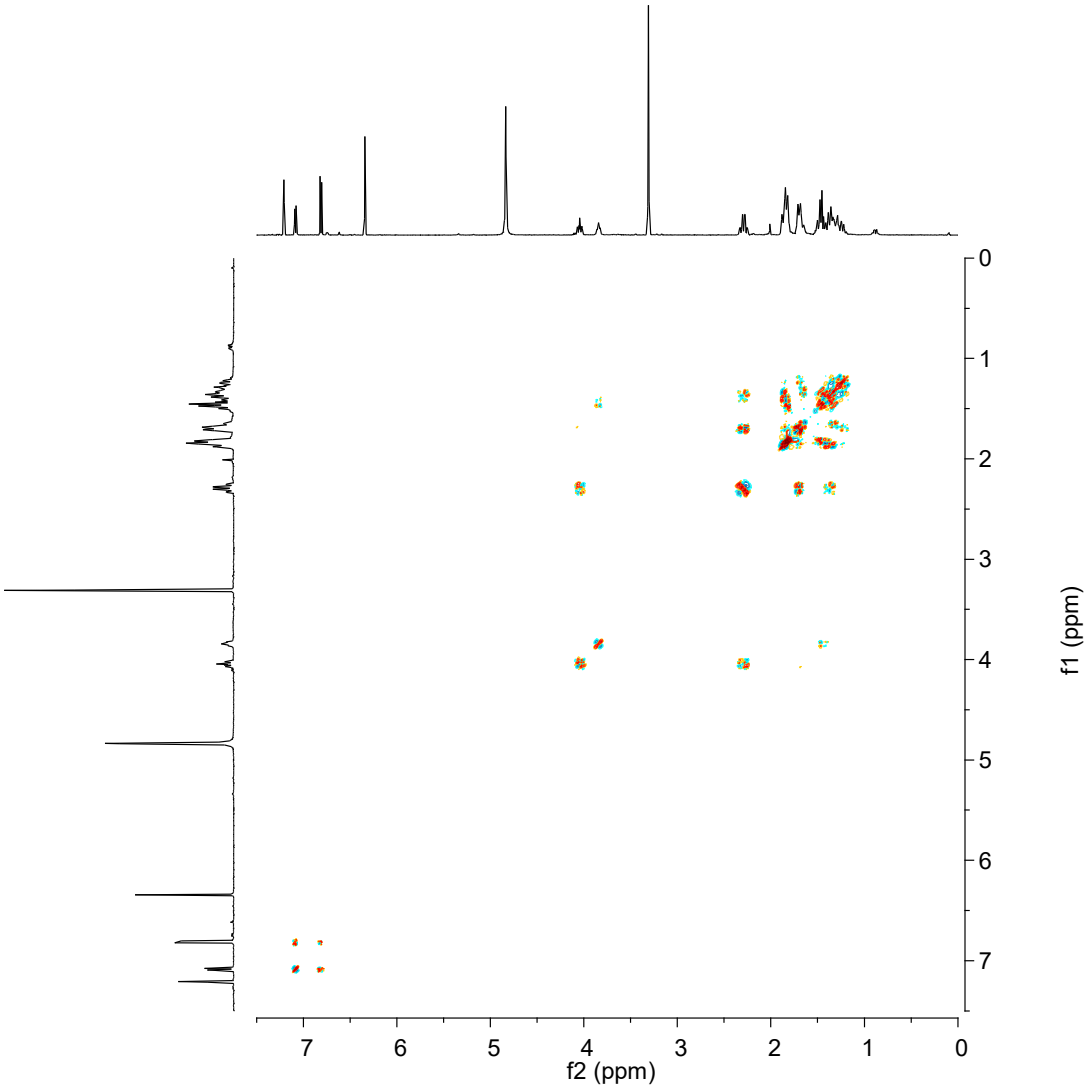

Figure S7. gDQF-COSY spectrum of **11**.

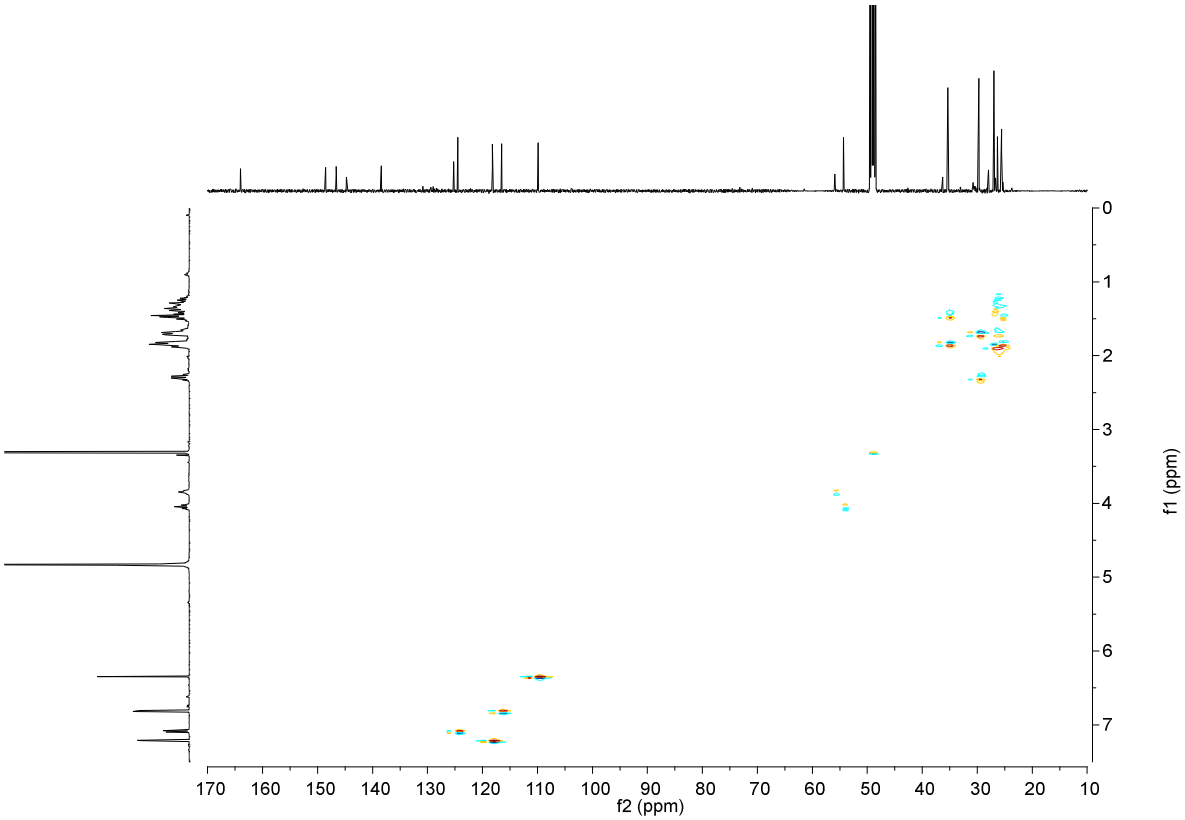

Figure S8. gHSQCAD spectrum of **11**.

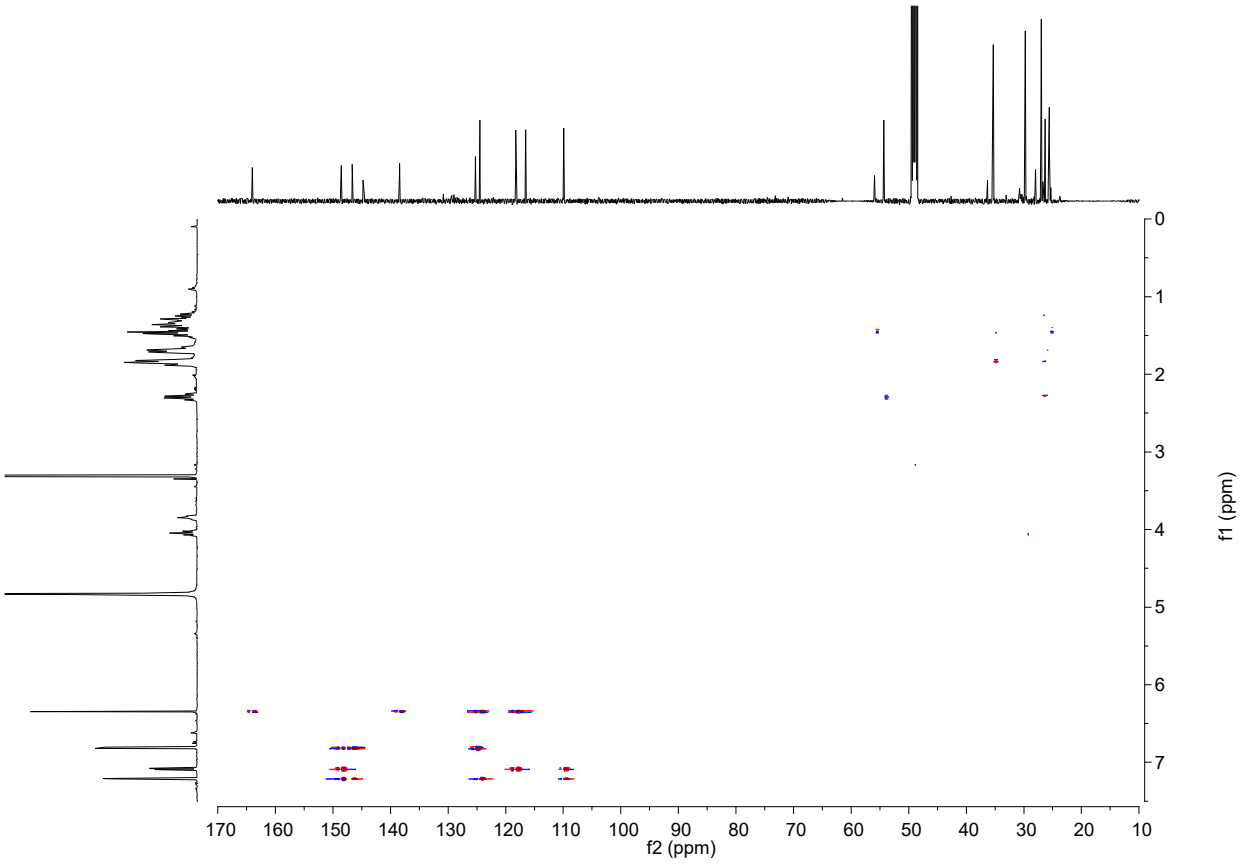

Figure S9. gHMBCAD spectrum of **11**.

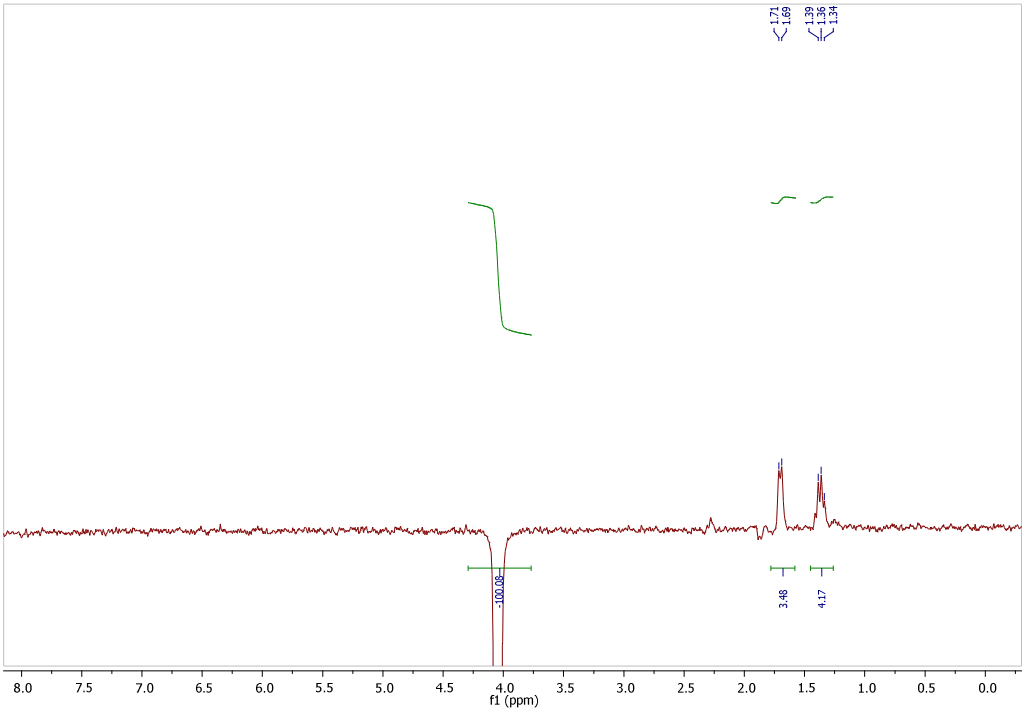

Figure S10. 1D NOESY of **11** irradiated at 4.05 ppm.

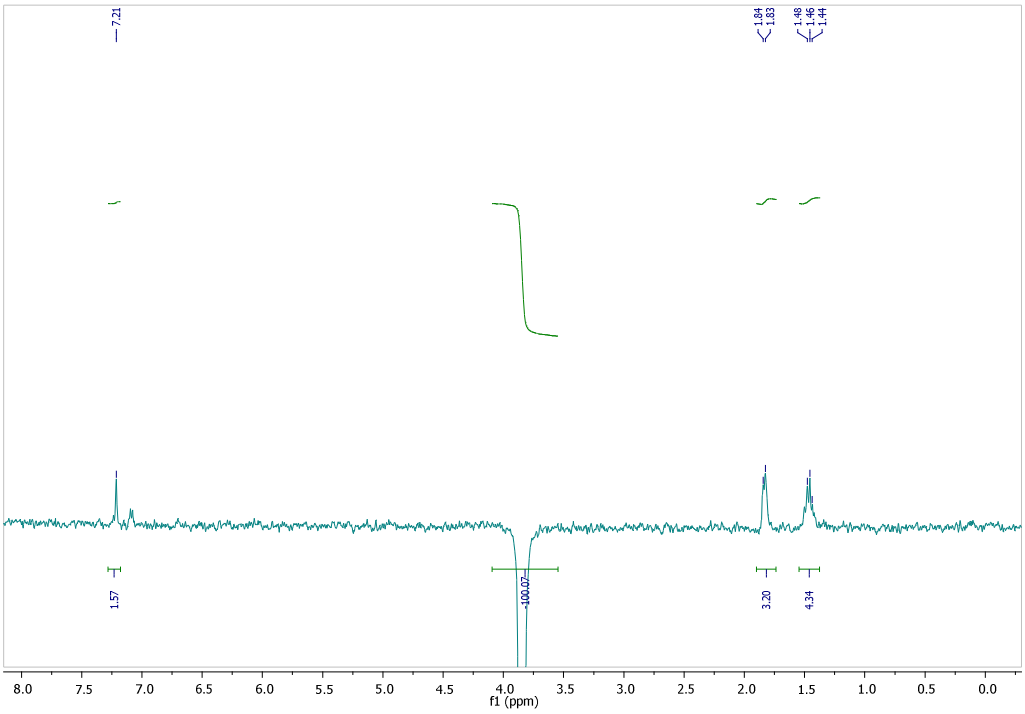

Figure S11. 1D NOESY of **11** irradiated at 3.85 ppm.

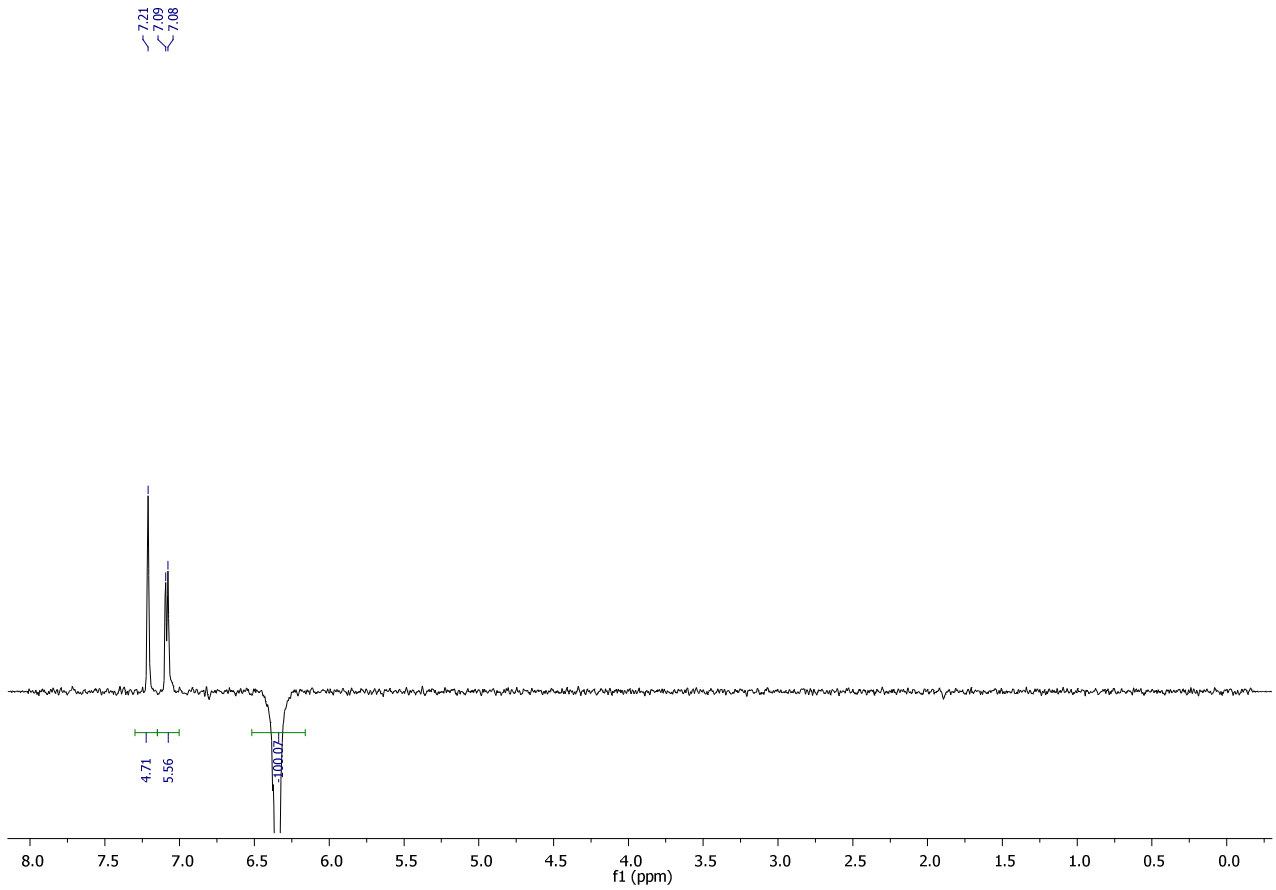

Figure S12. 1D NOESY of **11** irradiated at 6.35 ppm.

Spectroscopic characterization of 12

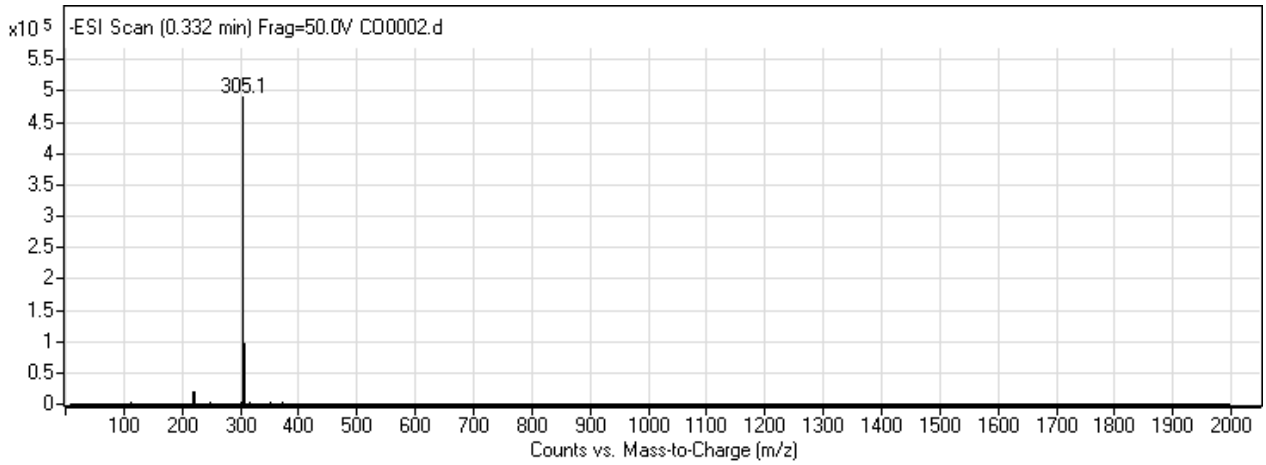

Figure S13. ESI MS spectrum of **12**.

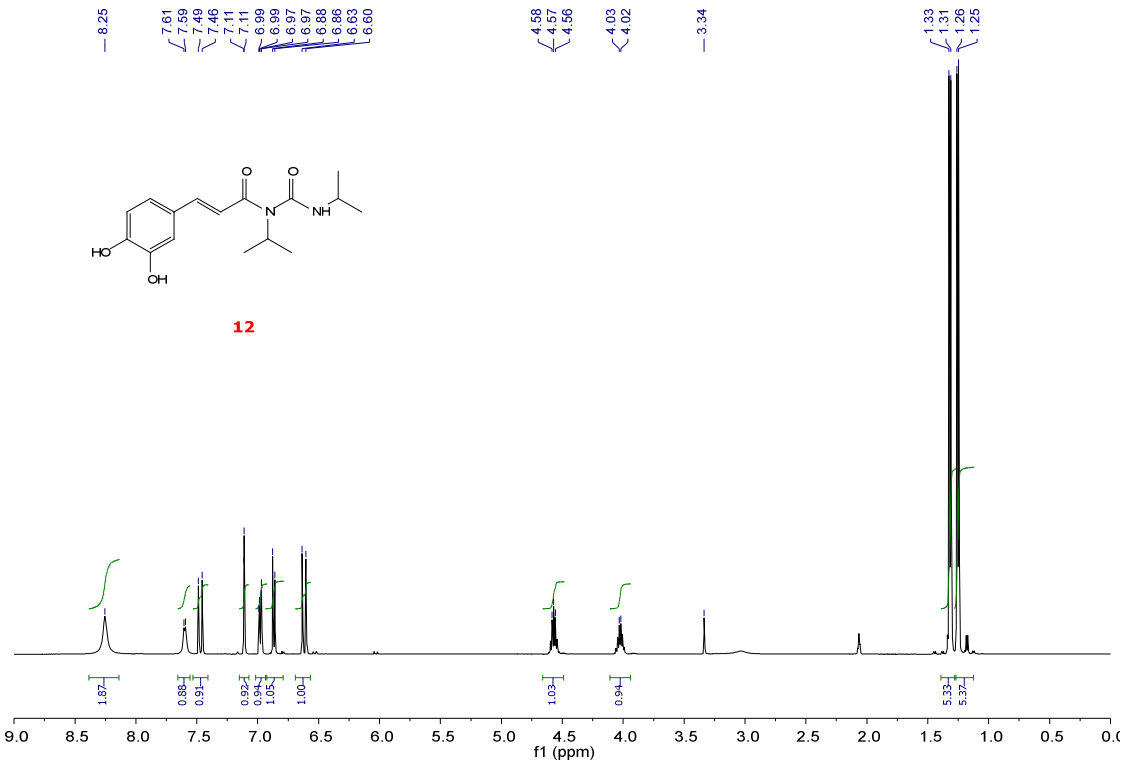

Figure S14. ^{1}H NMR spectrum (500 MHz, CD_3COCD_3) of **12**.

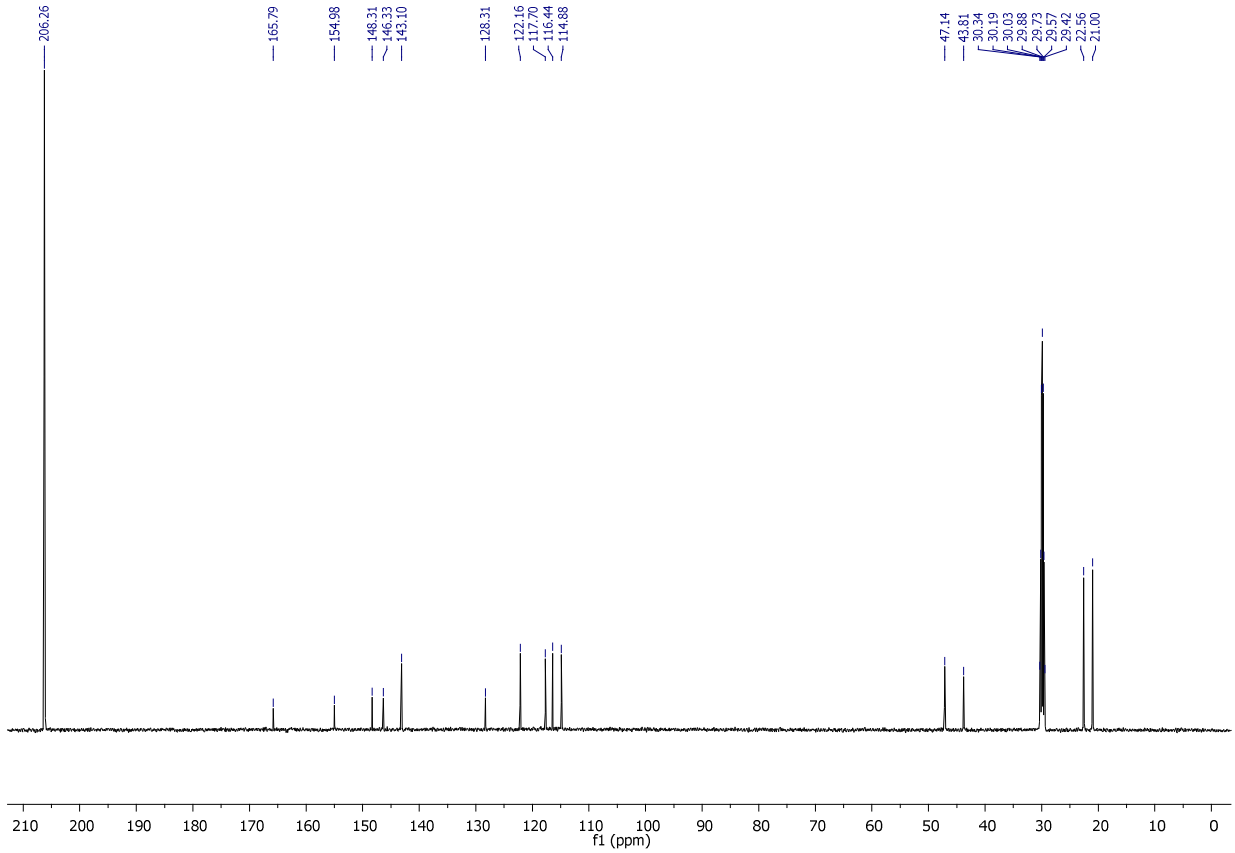

Figure S15. ^{13}C NMR spectrum (125 MHz, CD_3COCD_3) of **12**.

Spectroscopic characterization of 13

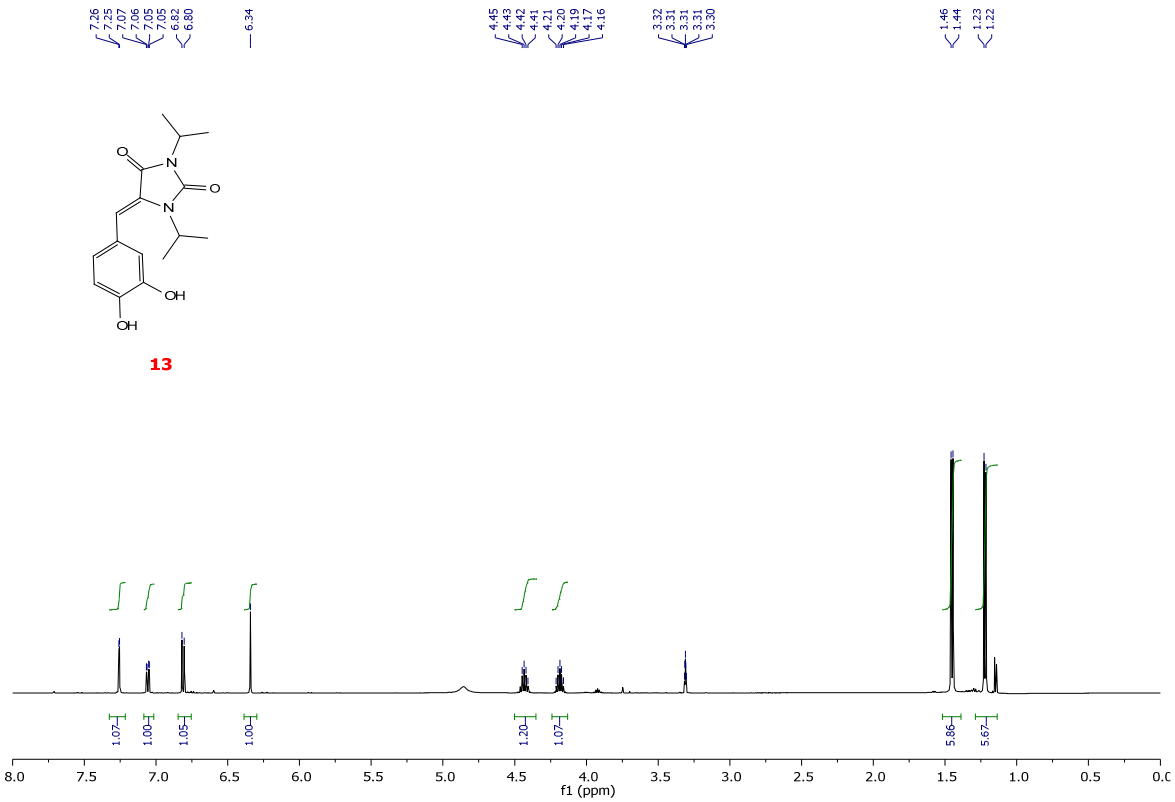

Figure S16. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **13**.

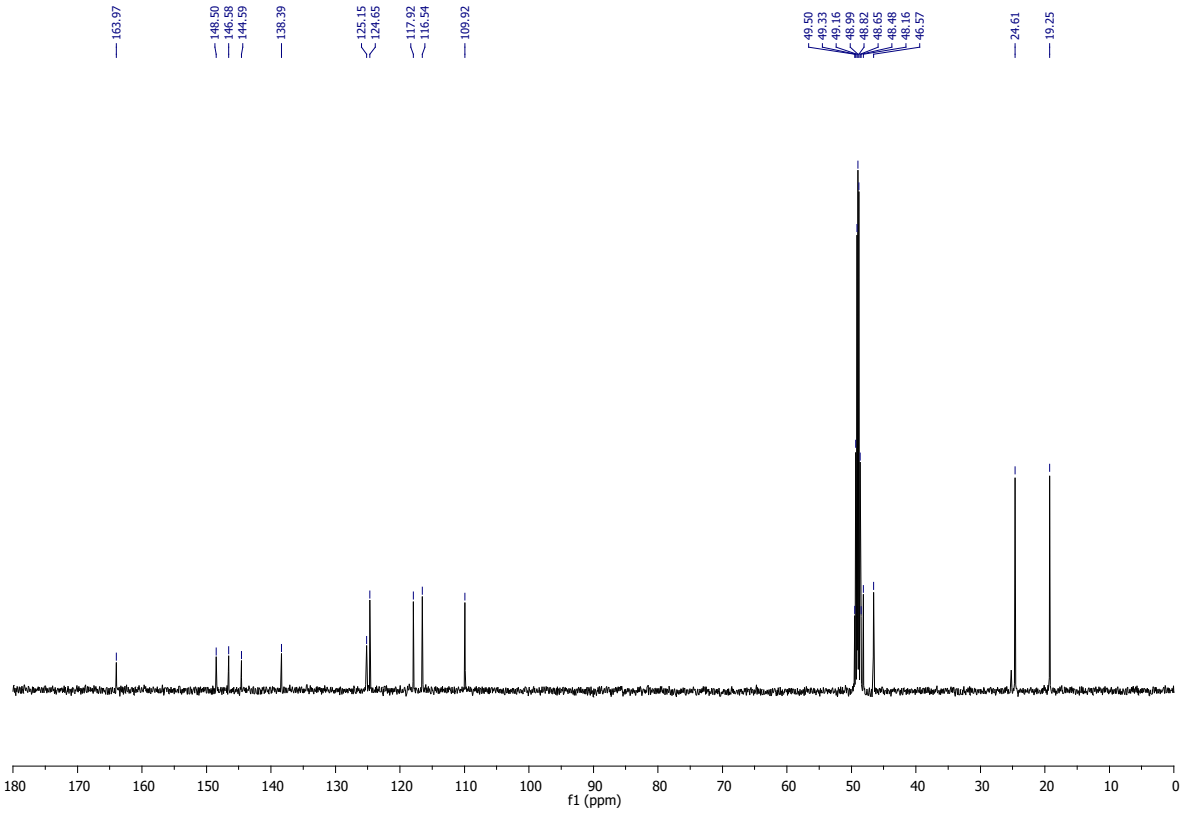

Figure S17. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **13**.

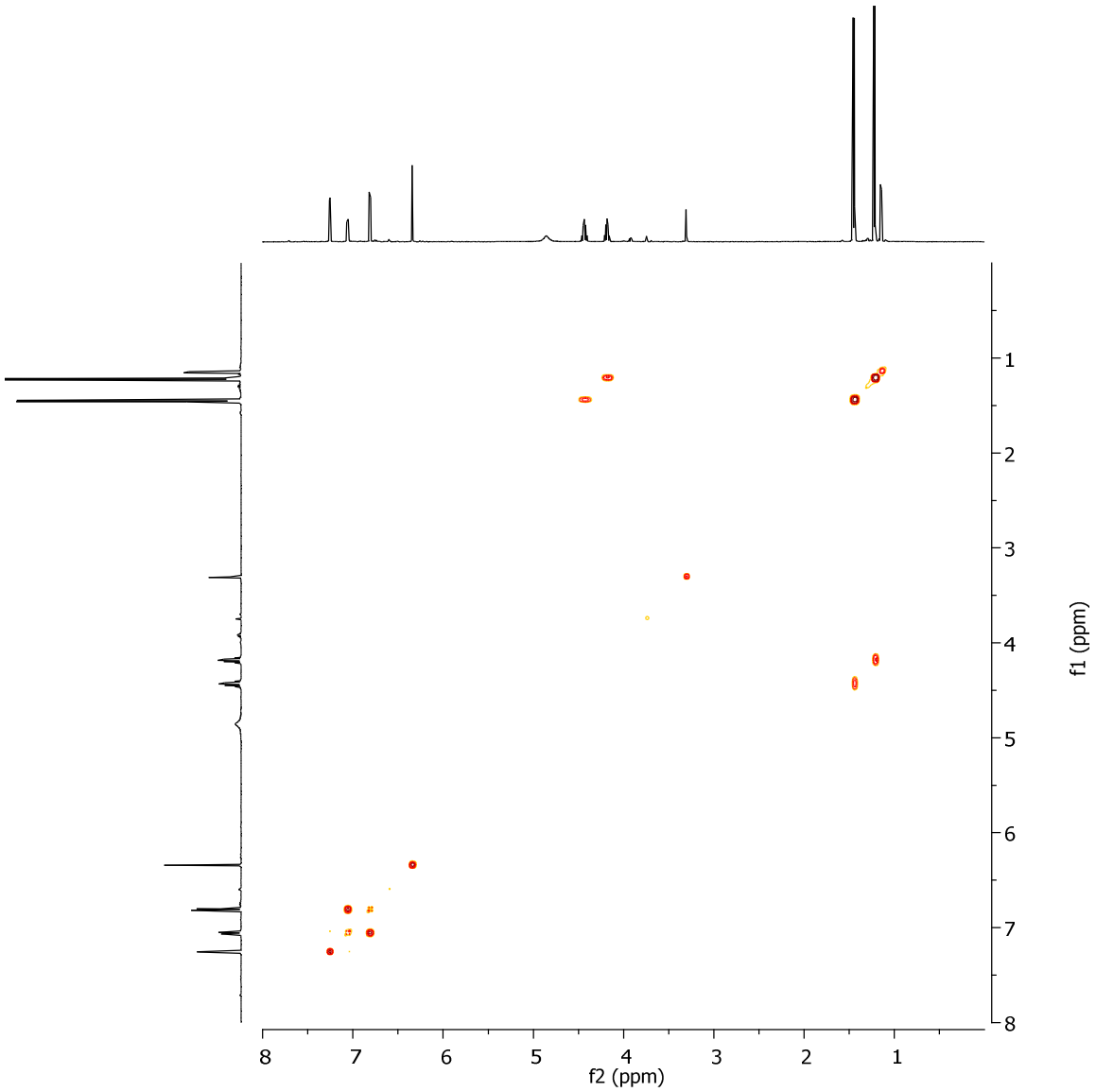

Figure S18. gCOSY spectrum of **13**.

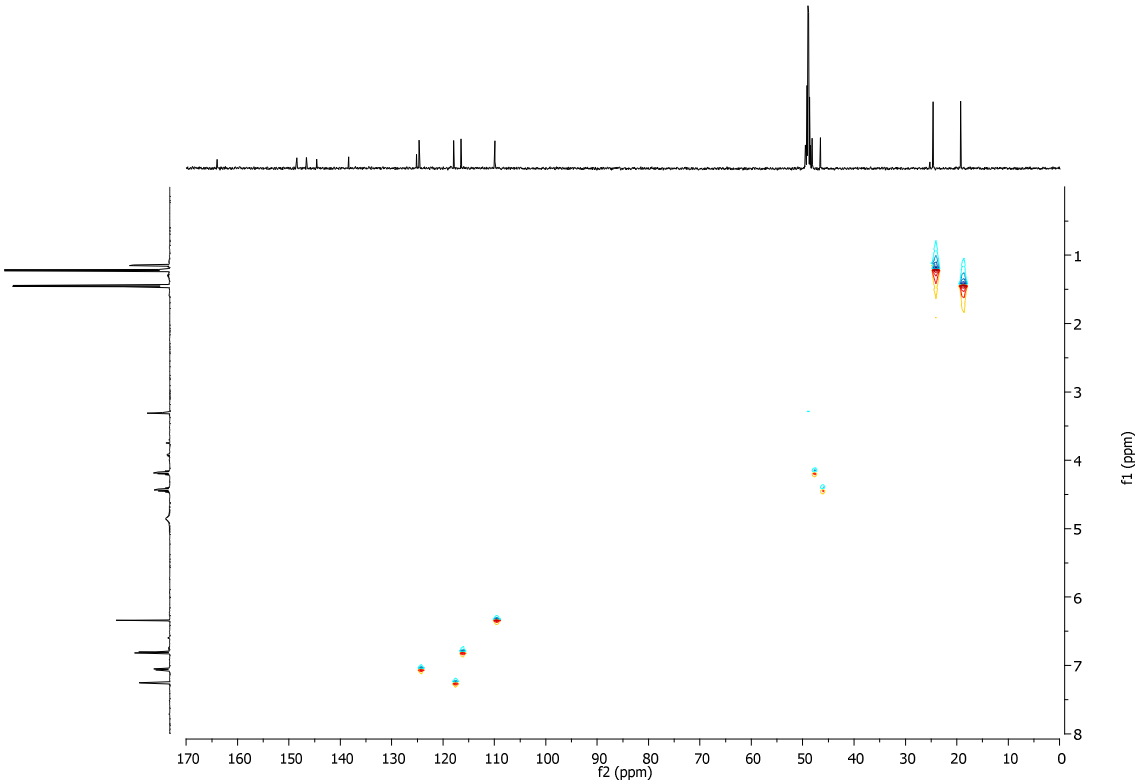

Figure S19. gHSCQAD spectrum of **13**.

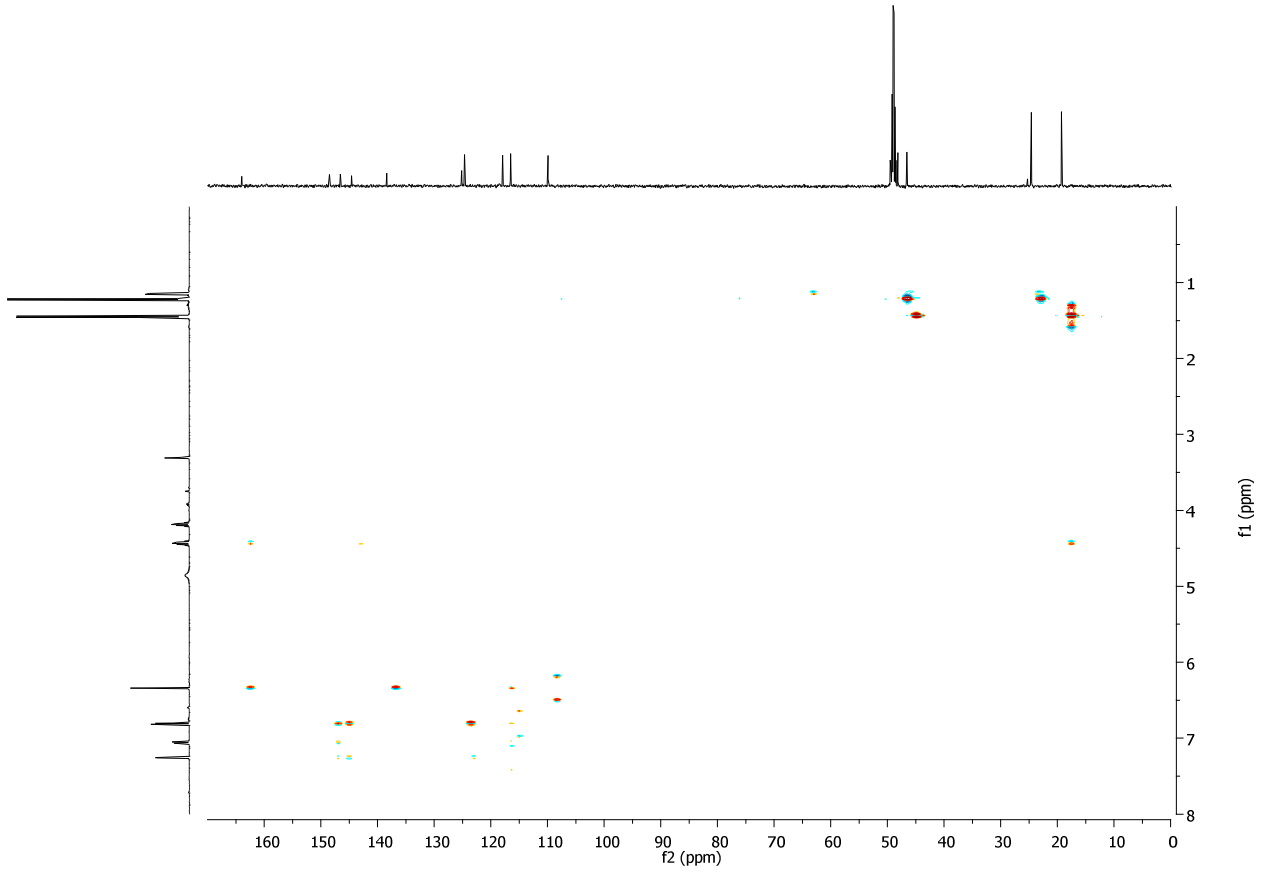

Figure S20. gHMBCAD spectrum of **13**.

Spectroscopic characterization of 16

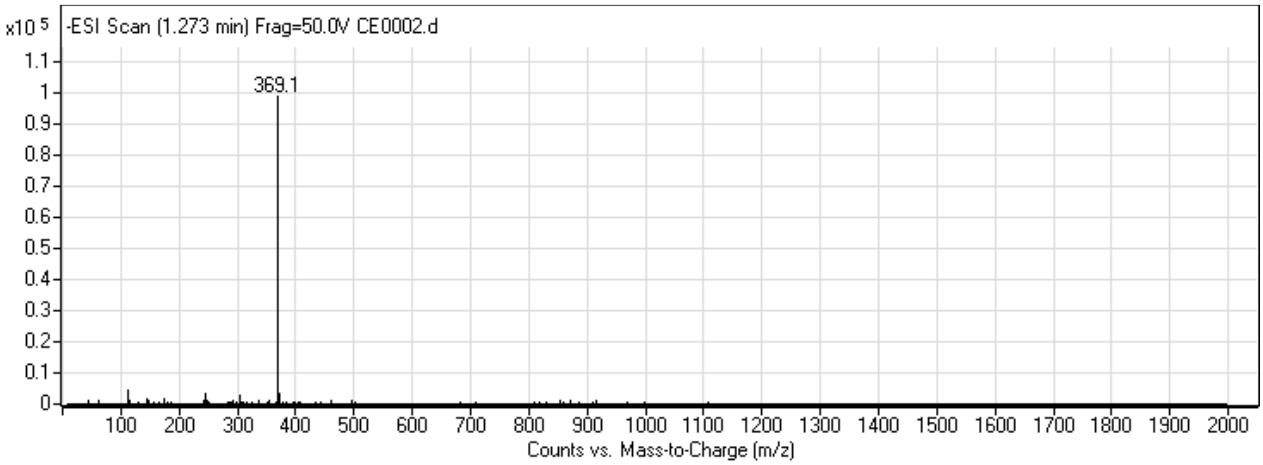

Figure S21. ESI MS spectrum of **16**.

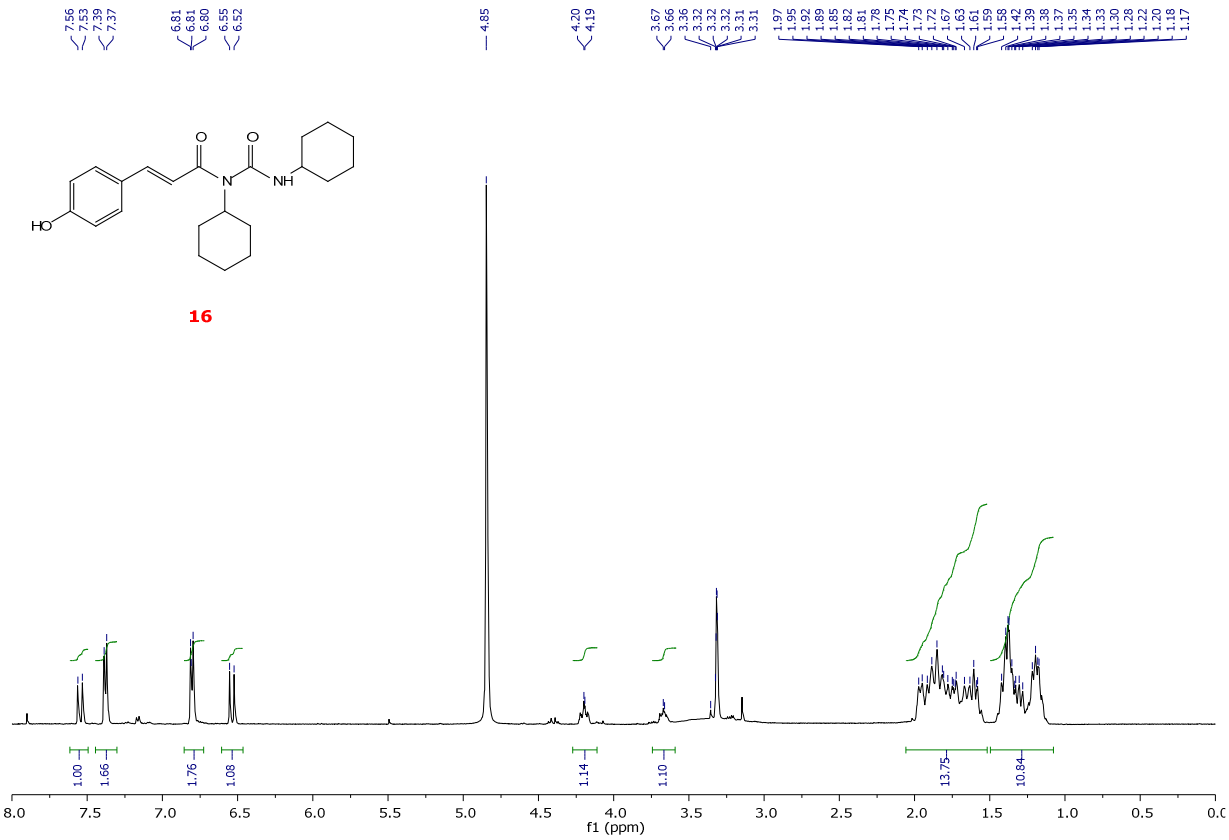

Figure S22. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **16**.

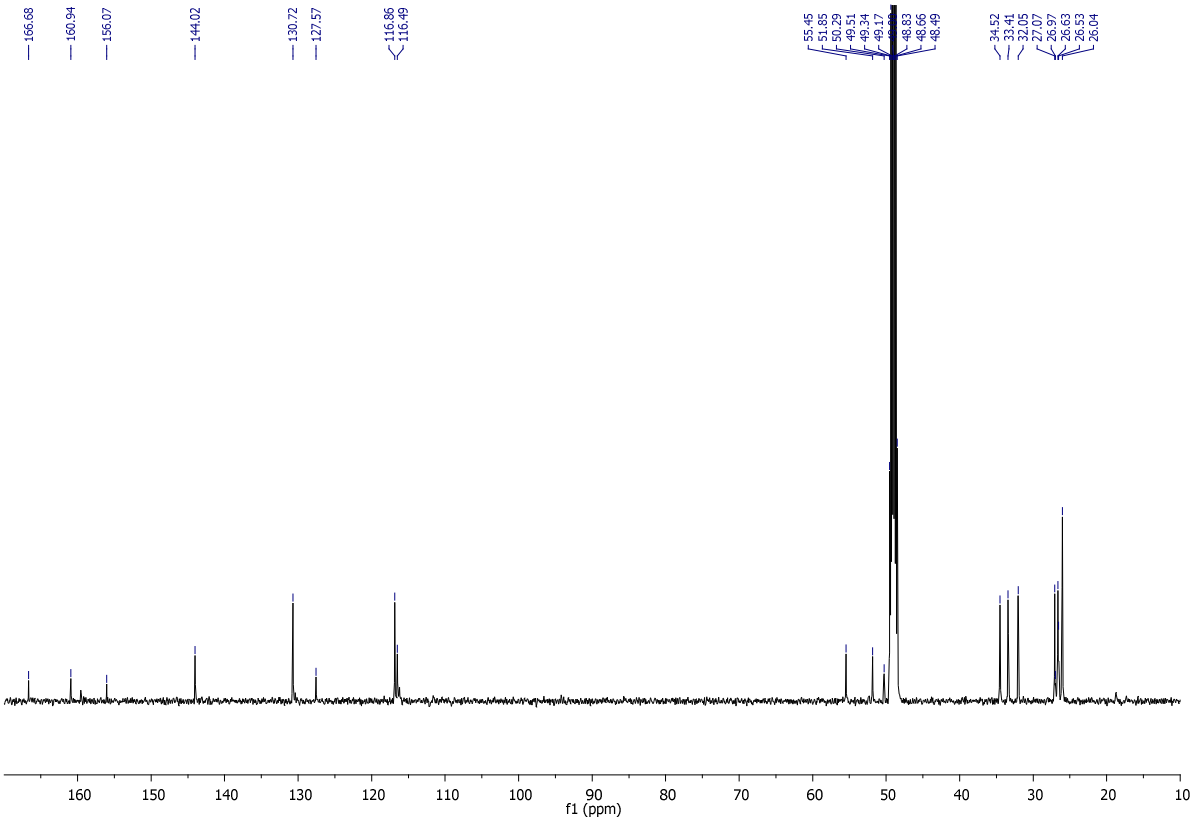

Figure S23. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **16**.

Spectroscopic characterization of 17

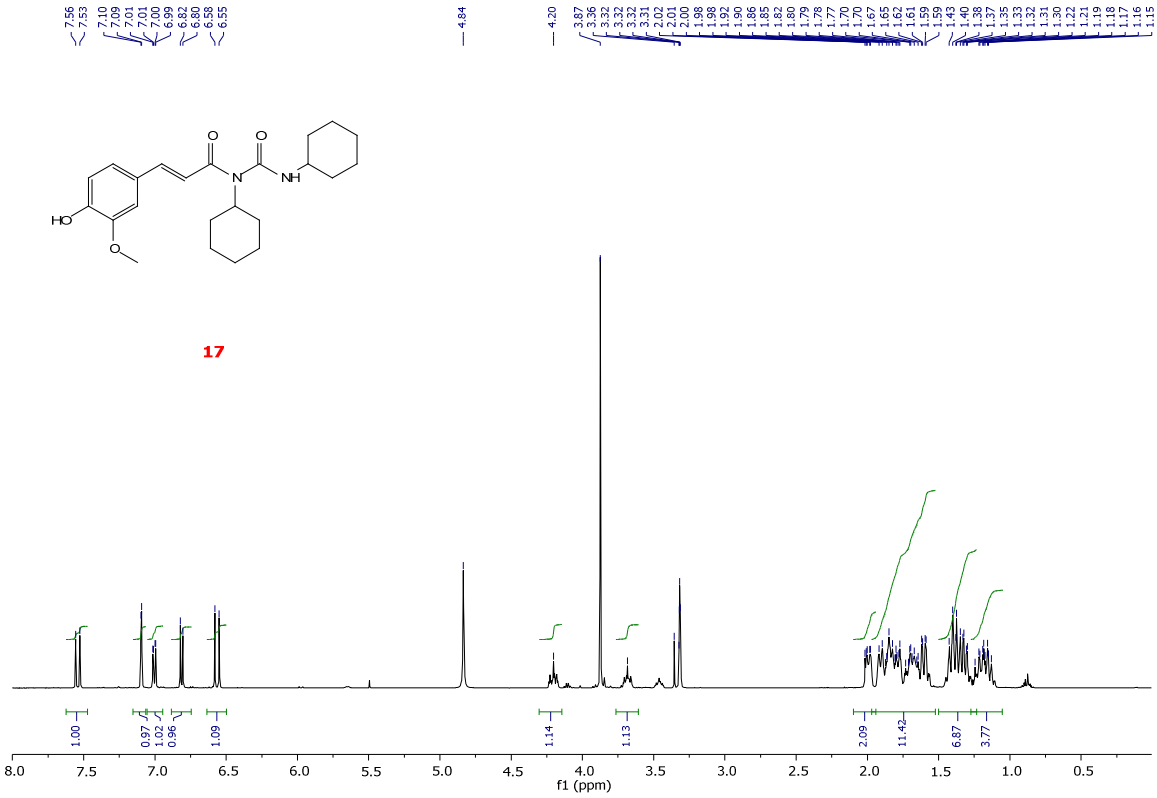

Figure S24. ^{1}H NMR spectrum (500 MHz, CD_3OD) of **17**.

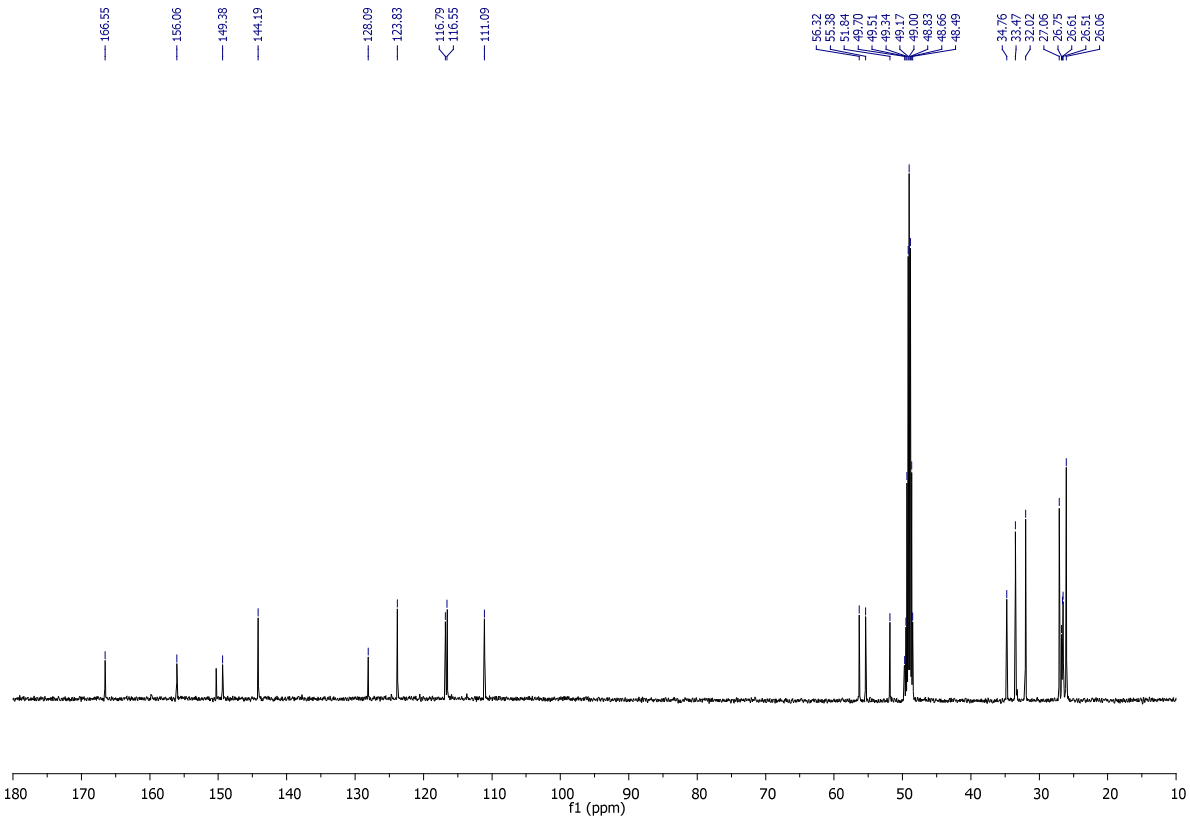

Figure S25. ^{13}C NMR spectrum (125 MHz, CD_3OD) of **14**.

General procedure for reaction screening

Some parameters such as solvent, enzyme concentration and pH have been screened in order to find the best reaction conditions to obtain the hydantoin **11** starting from **10**. The experiments performed have been summarized in Table S1. The urea **10** (2 mg; 0.05 mmol) was solubilized in the organic solvent (1mL), then adding the TvL solution (7 U/mL or 15 U/mL), previously prepared using acetate (0.1 M; pH 4.7) or phosphate (0.1 M; pH 7.0) buffer. Each mixture was stirred at room temperature in uncapped vials for 6-24 h. For each experiment, a blank was carried out in the same conditions, without enzyme. The reactions (100 µL, diluted to a final volume of 600 µL) were monitored at regular time intervals by HPLC (Agilent Series 1200) equipped with a diode array detector (DAD; G1315D). An analytical reversed phase column (Luna C_{18}, 5 µm; 4.6 × 250 mm; Phenomenex) was used to run reaction mixtures, eluting at 1 mL/min with the following gradient of CH_3CN/HCOOH (99:1 v/v; A) in H_2O/HCOOH (99:1 v/v; B): t_0 min A = 30%, t_{10} min A = 100%, t_{15} min A = 100%, t_{20} min A = 30%.

Table S1 Optimization of the reaction conditions for the synthesis of Hydantoin **11**[a]

Entry	Solvent	TvL (U/mL)	Time (h)	Conversion (%)[b]	Yield (%)[b]
1	EtOAc/buffer pH 4.7	7	1	92	38
		7	2	100	72
		7	6	100	65
2	EtOAc/buffer pH 4.7	15	1	98	40
		15	2	100	68
		15	6	100	62
3	EtOAc/buffer pH 7.0	7	2	45	5
		7	6	77	20
		7	24	90	25
4	CH_2Cl_2/buffer pH 4.7	7	1	89	8
		7	2	98	20
		7	6	100	28
5	CH_2Cl_2/buffer pH 4.7	15	1	94	12
		15	2	100	25
		15	6	100	29
6	CH_2Cl_2/buffer pH 7.0	7	2	20	0
		7	6	50	10
		7	24	85	12
7	buffer pH 4.7	7	2	70	5
		7	24	100	15
8	buffer pH 4.7	15	2	80	5
		15	24	100	10
9	buffer pH 7.0	7	2	40	0
		7	24	75	12
10	Acetone/buffer pH 4.7	7	2	100	13
		7	6	100	19
		7	24	100	18
11	Acetone/buffer pH 4.7	15	2	100	7
		15	6	100	10
		15	24	100	20
12	EtOH/buffer pH 4.7	7	2	100	12
		7	6	100	23
		7	24	100	25
13	EtOH/buffer pH 4.7	15	2	100	10
		15	6	100	19
		15	24	100	32

[a] Conditions: caffeoyl urea **10** (2mg/mL); the reactions were carried out at room temperature in uncapped vials.
[b]The yield was determined by HPLC-UV.

Cartesian coordinates, energies, and frequencies for compounds and transition states, in water-saturated ethyl acetate, at M06-2X level of theory

R

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.335939	0.109693	0.089646
2	8	0	-6.127758	-0.099641	0.251256
3	1	0	1.681942	2.412879	-0.472592
4	1	0	6.441818	-0.831743	0.792299
5	1	0	-0.305317	-1.788559	-0.465996
6	1	0	-2.445813	-2.618587	0.372105
7	1	0	-4.896852	-2.398585	0.595053
8	1	0	-1.971849	1.553961	-0.643378
9	1	0	3.249413	2.652664	0.327531
10	6	0	2.334708	2.067234	0.330975
11	6	0	-4.033600	0.952605	-0.233593
12	8	0	2.025287	-1.489353	-0.267177
13	6	0	4.145742	0.432401	0.087160
14	7	0	2.720888	0.668662	0.117503
15	6	0	-2.061537	-0.513999	-0.109756
16	6	0	1.766467	-0.312484	-0.037561
17	8	0	-4.532152	2.038860	-0.421430
18	6	0	-0.619476	-0.783567	-0.189156
19	6	0	-2.933689	-1.659237	0.220866
20	6	0	-2.584729	0.709310	-0.344437
21	1	0	3.856398	-1.549800	-0.273871
22	1	0	0.077723	1.105396	0.428372
23	8	0	4.912991	1.363218	0.257495
24	1	0	1.836751	2.195261	1.295135
25	1	0	6.119620	-2.163645	-0.345037
26	6	0	-4.264057	-1.553554	0.345743
27	1	0	6.463688	-0.523691	-0.948582
28	6	0	-4.934112	-0.252152	0.141427
29	7	0	4.551535	-0.829851	-0.128526
30	6	0	5.974774	-1.099900	-0.158817

0 imaginary frequencies

Zero-point correction=	0.231042 (Hartree/Particle)
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Thermal correction to Gibbs Free Energy=	0.184462
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Sum of electronic and thermal Energies=	-874.614660
Sum of electronic and thermal Enthalpies=	-874.613715
Sum of electronic and thermal Free Energies=	-874.677987

RH1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	6	0	-2.004023	-0.519896	0.085643
5	6	0	-0.592358	-0.777169	0.133846
6	6	0	0.366733	0.137094	-0.095034
7	6	0	1.806864	-0.317399	-0.066809
8	7	0	2.733675	0.642984	0.160160
9	6	0	4.176507	0.435049	0.062499
10	7	0	4.586259	-0.805749	-0.206859
11	6	0	6.013028	-1.057864	-0.330944
12	8	0	4.901369	1.386666	0.220623
13	6	0	2.336350	2.008894	0.521432
14	8	0	2.015100	-1.500214	-0.269902
15	6	0	-2.865679	-1.687417	0.340679
16	6	0	-4.197519	-1.617455	0.323925
17	6	0	-4.832844	-0.324430	0.042114
18	8	0	-6.014953	-0.114886	-0.005621
19	1	0	-1.931055	1.602855	-0.368169

20	1	0	-0.270691	-1.788897	0.349674
21	1	0	0.139024	1.163766	-0.346498
22	1	0	3.908466	-1.542441	-0.313410
23	1	0	6.156548	-2.113890	-0.535869
24	1	0	6.527770	-0.791131	0.590159
25	1	0	6.435462	-0.468135	-1.142359
26	1	0	3.213906	2.499279	0.926020
27	1	0	1.560042	1.989660	1.282271
28	1	0	2.006729	2.570864	-0.352433
29	1	0	-2.365477	-2.624678	0.543827
30	1	0	-4.844223	-2.464191	0.506776
31	1	0	-5.474187	1.850661	-0.431912

0 imaginary frequencies

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Thermal correction to Energy=	0.260584
Thermal correction to Enthalpy=	0.261528
Thermal correction to Gibbs Free Energy=	0.197232
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Sum of electronic and thermal Energies=	-874.997590
Sum of electronic and thermal Enthalpies=	-874.996646
Sum of electronic and thermal Free Energies=	-875.060941

RH1-TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.608061	1.851909	1.121020
2	6	0	3.176968	0.775827	0.539961
3	6	0	1.852330	0.462410	0.442494
4	6	0	1.483641	-0.730308	-0.202652
5	6	0	0.146875	-1.161895	-0.329783
6	6	0	-0.912960	-0.571308	0.294601
7	6	0	-2.255406	-1.259391	0.268569
8	7	0	-3.357128	-0.445798	0.212836
9	6	0	-3.221901	0.914290	-0.088753
10	7	0	-2.083304	1.151349	-0.871964
11	6	0	-1.745314	2.553957	-1.109380
12	8	0	-3.957106	1.770394	0.304924
13	6	0	-4.662373	-1.002980	0.574398
14	8	0	-2.308419	-2.456843	0.379433
15	6	0	2.502822	-1.612395	-0.793158
16	6	0	3.807844	-1.347731	-0.720182
17	6	0	4.250727	-0.123723	-0.040381
18	8	0	5.394795	0.225578	0.091224
19	1	0	1.120495	1.141662	0.853619
20	1	0	-0.049554	-2.052730	-0.913270
21	1	0	-0.778957	0.214051	1.026306
22	1	0	-2.045995	0.568661	-1.698802
23	1	0	-0.808914	2.598911	-1.658585
24	1	0	-1.637918	3.058140	-0.152760
25	1	0	-2.529609	3.058719	-1.673144
26	1	0	-5.368991	-0.181708	0.623536
27	1	0	-4.590961	-1.496049	1.540256
28	1	0	-4.968171	-1.730982	-0.173215
29	1	0	2.147586	-2.508218	-1.284563
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31	1	0	4.584795	1.871511	1.074509

1 imaginary frequency: -133.3289

Zero-point correction=	0.243405 (Hartree/Particle)
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Thermal correction to Enthalpy=	0.261206
Thermal correction to Gibbs Free Energy=	0.197433
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Sum of electronic and thermal Enthalpies=	-874.991963
Sum of electronic and thermal Free Energies=	-875.055737

PH1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

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3	6	0	-1.846409	0.401930	-0.542810
4	6	0	-1.321716	-0.656554	0.291149
5	6	0	-0.008239	-0.939349	0.429781
6	6	0	1.084016	-0.196547	-0.252912
7	6	0	2.303637	-1.048398	-0.591435
8	7	0	3.452431	-0.347963	-0.203387
9	6	0	3.211180	0.807769	0.446806
10	7	0	1.691024	0.900625	0.604829
11	6	0	1.185804	2.283215	0.349781
12	8	0	3.916709	1.650024	0.878615
13	6	0	4.800871	-0.847560	-0.479838
14	8	0	2.303017	-2.112700	-1.114720
15	6	0	-2.268619	-1.490024	1.046359
16	6	0	-3.586357	-1.291888	1.003479
17	6	0	-4.141881	-0.214649	0.178328
18	8	0	-5.319534	0.040724	0.081378
19	1	0	-1.198013	1.022595	-1.145786
20	1	0	0.294304	-1.775809	1.048003
21	1	0	0.752755	0.279363	-1.175977
22	1	0	1.495897	0.673154	1.585227
23	1	0	0.121137	2.296105	0.567266
24	1	0	1.370910	2.523739	-0.693913
25	1	0	1.729221	2.966363	0.995297
26	1	0	5.510677	-0.186864	0.007753
27	1	0	4.964854	-0.858430	-1.554122
28	1	0	4.882425	-1.858414	-0.089818
29	1	0	-1.850163	-2.285551	1.649401
30	1	0	-4.289334	-1.899486	1.555629
31	1	0	-4.683763	1.515310	-1.221001

0 imaginary frequencies

Zero-point correction=	0.246954	(Hartree/Particle)
Thermal correction to Energy=	0.261846	
Thermal correction to Enthalpy=	0.262790	
Thermal correction to Gibbs Free Energy=	0.204261	
Sum of electronic and zero-point Energies=	-875.049664	
Sum of electronic and thermal Energies=	-875.034772	
Sum of electronic and thermal Enthalpies=	-875.033828	
Sum of electronic and thermal Free Energies=	-875.092357	

*Z-**P**-exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.317787	-0.467549	-0.073950
2	6	0	-2.624288	-1.179336	-0.229812
3	7	0	-3.583912	-0.208458	-0.059661
4	6	0	-3.013920	1.025804	0.243673
5	7	0	-1.638780	0.864113	0.191913
6	6	0	-0.768873	1.858648	0.790128
7	6	0	-5.007655	-0.446722	-0.135170
8	6	0	-0.151657	-1.105367	-0.189922
9	6	0	1.200262	-0.537820	-0.224412
10	6	0	1.493030	0.582430	-0.996853
11	6	0	2.787685	1.083198	-1.049060
12	6	0	3.795033	0.467967	-0.332856
13	6	0	3.520566	-0.670375	0.431530
14	6	0	2.234585	-1.169205	0.472494
15	8	0	-2.827145	-2.341226	-0.470369
16	8	0	-3.611384	2.034223	0.516274
17	8	0	5.098799	0.881035	-0.315141
18	8	0	4.510113	-1.282677	1.124317
19	1	0	5.331960	-0.803186	0.969311
20	1	0	2.043775	-2.053443	1.065736
21	1	0	-0.249287	-2.180403	-0.297545
22	1	0	-0.091121	1.375642	1.492537
23	1	0	-5.509711	0.496211	0.061135
24	1	0	0.713743	1.042521	-1.588247
25	1	0	3.016484	1.948634	-1.659444
26	1	0	5.211998	1.650853	-0.877864
27	1	0	-0.179524	2.384428	0.042061
28	1	0	-1.402494	2.572160	1.310156

29	1	0	-5.300536	-1.188331	0.605456
30	1	0	-5.271375	-0.815548	-1.124447

0 imaginary frequencies

Zero-point correction=	0.233169 (Hartree/Particle)
Thermal correction to Energy=	0.250081
Thermal correction to Enthalpy=	0.251026
Thermal correction to Gibbs Free Energy=	0.187657
Sum of electronic and zero-point Energies=	-874.700967
Sum of electronic and thermal Energies=	-874.684055
Sum of electronic and thermal Enthalpies=	-874.683111
Sum of electronic and thermal Free Energies=	-874.746480

E-**P**-*exo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.291135	-0.477919	-0.000404
2	6	0	1.616781	0.982461	-0.000719
3	7	0	2.991100	1.043828	-0.000149
4	6	0	3.573556	-0.221860	-0.000426
5	7	0	2.538434	-1.121022	-0.000430
6	6	0	2.748868	-2.545044	-0.000177
7	6	0	3.769803	2.261834	0.000532
8	6	0	0.129509	-1.154476	-0.000125
9	6	0	-1.272865	-0.762678	0.000028
10	6	0	-2.212926	-1.798493	0.000438
11	6	0	-3.573765	-1.543887	0.000621
12	6	0	-4.029677	-0.238074	0.000391
13	6	0	-3.099190	0.805916	-0.000035
14	6	0	-1.746440	0.556795	-0.000217
15	8	0	0.887888	1.947684	-0.000079
16	8	0	4.756822	-0.450663	-0.000003
17	8	0	-5.354909	0.026435	0.000569
18	8	0	-3.641627	2.062674	-0.000270
19	1	0	-2.940201	2.719586	-0.000254
20	1	0	-1.049511	1.381784	-0.000556
21	1	0	0.254487	-2.232480	0.000011
22	1	0	3.821773	-2.714950	-0.000131
23	1	0	3.071390	3.093632	0.000259
24	1	0	-1.869955	-2.824743	0.000622
25	1	0	-4.298052	-2.345948	0.000947
26	1	0	-5.471061	0.984082	0.000397
27	1	0	2.308662	-3.000020	0.888522
28	1	0	4.400938	2.301494	0.885840
29	1	0	4.401959	2.301752	-0.884033
30	1	0	2.308701	-3.000318	-0.888742

0 imaginary frequencies

Zero-point correction=	0.233204 (Hartree/Particle)
Thermal correction to Energy=	0.249249
Thermal correction to Enthalpy=	0.250193
Thermal correction to Gibbs Free Energy=	0.189302
Sum of electronic and zero-point Energies=	-874.701860
Sum of electronic and thermal Energies=	-874.685815
Sum of electronic and thermal Enthalpies=	-874.684871
Sum of electronic and thermal Free Energies=	-874.745762

RH2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	4.409829	2.147165	-0.633920
2	6	0	4.016154	1.052383	-0.343248
3	6	0	2.575139	0.716294	-0.363356
4	6	0	2.144841	-0.507250	-0.006779
5	6	0	0.725922	-0.851249	-0.034544
6	6	0	-0.283627	0.025954	0.096320
7	6	0	-1.647425	-0.442340	-0.008627
8	7	0	-2.697625	0.366599	0.281675
9	6	0	-4.016321	-0.086462	-0.024586
10	7	0	-4.999344	0.795531	0.050709

11	6	0	-6.369951	0.385050	-0.264205
12	8	0	-4.200225	-1.263382	-0.346084
13	6	0	-2.508706	1.684025	0.905882
14	8	0	-1.857129	-1.634578	-0.401445
15	6	0	3.090777	-1.570392	0.375384
16	6	0	4.409234	-1.377000	0.424176
17	6	0	4.998979	-0.065785	0.081471
18	8	0	6.175572	0.155776	0.118472
19	1	0	1.911634	1.500817	-0.704324
20	1	0	0.481195	-1.902215	-0.150085
21	1	0	-0.094768	1.073721	0.261871
22	1	0	-4.806795	1.771063	0.196318
23	1	0	-7.034808	1.200569	-0.001425
24	1	0	-6.622970	-0.497443	0.316428
25	1	0	-6.463308	0.154873	-1.323216
26	1	0	-3.322000	1.853051	1.605876
27	1	0	-2.476431	2.475496	0.158431
28	1	0	-1.593613	1.683494	1.484696
29	1	0	2.673208	-2.537471	0.627195
30	1	0	5.098809	-2.159642	0.709095
31	1	0	-2.905850	-1.770431	-0.431047

0 imaginary frequencies

Zero-point correction=	0.242848 (Hartree/Particle)
Thermal correction to Energy=	0.259329
Thermal correction to Enthalpy=	0.260273
Thermal correction to Gibbs Free Energy=	0.197612
Sum of electronic and zero-point Energies=	-875.030813
Sum of electronic and thermal Energies=	-875.014333
Sum of electronic and thermal Enthalpies=	-875.013389
Sum of electronic and thermal Free Energies=	-875.076050

RH2-TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.856635	-1.585782	1.271781
2	6	0	3.247556	-0.872434	0.526684
3	6	0	1.777827	-0.997509	0.366037
4	6	0	1.105225	-0.189017	-0.471463
5	6	0	-0.350840	-0.296819	-0.615709
6	6	0	-1.079004	-1.456248	-0.304188
7	6	0	-2.446065	-1.329377	-0.184340
8	7	0	-3.071835	-0.118471	-0.121465
9	6	0	-2.441359	1.075673	0.302042
10	7	0	-1.130323	0.944612	0.847311
11	6	0	-0.469076	2.215541	1.172398
12	8	0	-2.959409	2.138310	0.169510
13	6	0	-4.525779	-0.047208	-0.383835
14	8	0	-3.282180	-2.341188	-0.086078
15	6	0	1.791120	0.858891	-1.245720
16	6	0	3.108556	1.057660	-1.178052
17	6	0	3.960021	0.225214	-0.300102
18	8	0	5.144453	0.370013	-0.205418
19	1	0	1.300211	-1.761203	0.967253
20	1	0	-0.784242	0.382487	-1.343881
21	1	0	-0.597826	-2.385870	-0.042610
22	1	0	-1.080107	0.257365	1.593852
23	1	0	0.536933	1.988880	1.515673
24	1	0	-1.015164	2.762304	1.938550
25	1	0	-0.424663	2.825524	0.274187
26	1	0	-4.773908	0.988038	-0.580575
27	1	0	-5.079475	-0.411329	0.477814
28	1	0	-4.755636	-0.657671	-1.250651
29	1	0	1.182549	1.472043	-1.899941
30	1	0	3.609429	1.822757	-1.755385
31	1	0	-2.848083	-3.183342	-0.276074

1 imaginary frequency: -482.6322

Zero-point correction=	0.242977 (Hartree/Particle)
Thermal correction to Energy=	0.259044
Thermal correction to Enthalpy=	0.259988
Thermal correction to Gibbs Free Energy=	0.197971

Sum of electronic and zero-point Energies=	-874.980604
Sum of electronic and thermal Energies=	-874.964538
Sum of electronic and thermal Enthalpies=	-874.963594
Sum of electronic and thermal Free Energies=	-875.025611

PH2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.643090	1.630325	1.420345
2	6	0	-3.131030	0.883215	0.636805
3	6	0	-1.662802	0.852083	0.430709
4	6	0	-1.107614	-0.011066	-0.428372
5	6	0	0.396943	-0.066401	-0.598425
6	6	0	1.067661	1.267004	-0.562992
7	6	0	2.375563	1.314876	-0.306072
8	7	0	3.116341	0.153668	-0.018856
9	6	0	2.534291	-0.997243	0.370275
10	7	0	1.010091	-0.889118	0.530951
11	6	0	0.418270	-2.251602	0.695210
12	8	0	3.044558	-2.040256	0.617010
13	6	0	4.589438	0.185920	-0.129261
14	8	0	3.164575	2.386306	-0.280834
15	6	0	-1.920877	-0.946815	-1.219464
16	6	0	-3.251509	-0.997557	-1.126051
17	6	0	-3.982332	-0.103007	-0.200199
18	8	0	-5.173434	-0.119847	-0.081244
19	1	0	-1.087471	1.566042	1.008995
20	1	0	0.647649	-0.632262	-1.501957
21	1	0	0.501240	2.159857	-0.772233
22	1	0	0.843912	-0.350492	1.389811
23	1	0	-0.633495	-2.134761	0.933815
24	1	0	0.945890	-2.765624	1.489720
25	1	0	0.549379	-2.791646	-0.238321
26	1	0	4.949543	-0.830284	-0.023146
27	1	0	4.999105	0.816768	0.653965
28	1	0	4.861231	0.584952	-1.101435
29	1	0	-1.402583	-1.600687	-1.911377
30	1	0	-3.848887	-1.678247	-1.717296
31	1	0	2.692586	3.175882	-0.570385

0 imaginary frequencies

Zero-point correction=	0.246819 (Hartree/Particle)
Thermal correction to Energy=	0.263298
Thermal correction to Enthalpy=	0.264242
Thermal correction to Gibbs Free Energy=	0.201653
Sum of electronic and zero-point Energies=	-875.004365
Sum of electronic and thermal Energies=	-874.987886
Sum of electronic and thermal Enthalpies=	-874.986942
Sum of electronic and thermal Free Energies=	-875.049531

P-*endo*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.609517	-1.264812	-0.924643
2	6	0	-2.998438	-1.327844	-0.935177
3	6	0	-1.712278	0.586780	0.609970
4	6	0	-3.090124	0.522098	0.608221
5	8	0	-3.810901	1.384045	1.361531
6	8	0	-5.098468	-0.420990	-0.112173
7	6	0	-3.734592	-0.442684	-0.174878
8	6	0	-0.962791	-0.307554	-0.156559
9	6	0	0.512945	2.094685	-0.882087
10	8	0	3.125343	2.070115	-0.372071
11	8	0	3.316265	-2.364391	0.612605
12	6	0	4.678890	0.008444	0.298685
13	7	0	3.233941	-0.131895	0.152370
14	6	0	2.553520	1.016143	-0.193735
15	7	0	1.174716	0.904641	-0.347110
16	6	0	0.517308	-0.283835	-0.100610
17	6	0	1.203683	-1.396805	0.221128
18	6	0	2.645065	-1.391663	0.344125
19	1	0	-4.746824	1.181866	1.247759

20	1	0	-5.470232	-1.122803	-0.652367
21	1	0	-1.233389	1.330444	1.232640
22	1	0	-3.507938	-2.068060	-1.539864
23	1	0	-1.030372	-1.955079	-1.521238
24	1	0	-0.403429	1.801393	-1.381039
25	1	0	5.069372	-0.957176	0.596287
26	1	0	0.691769	-2.316754	0.448715
27	1	0	1.189093	2.569494	-1.585425
28	1	0	5.116406	0.325842	-0.645333
29	1	0	4.897743	0.764559	1.048675
30	1	0	0.287262	2.809103	-0.091414

0 imaginary frequencies

Zero-point correction=	0.234023 (Hartree/Particle)
Thermal correction to Energy=	0.250394
Thermal correction to Enthalpy=	0.251338
Thermal correction to Gibbs Free Energy=	0.189691
Sum of electronic and zero-point Energies=	-874.708241
Sum of electronic and thermal Energies=	-874.691870
Sum of electronic and thermal Enthalpies=	-874.690926
Sum of electronic and thermal Free Energies=	-874.752572