Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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Synthesis, structure prediction, pharmacokinetic properties, molecular docking and antitumor activities of some novel thiazinone derivatives.

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New Journal of Chemistry

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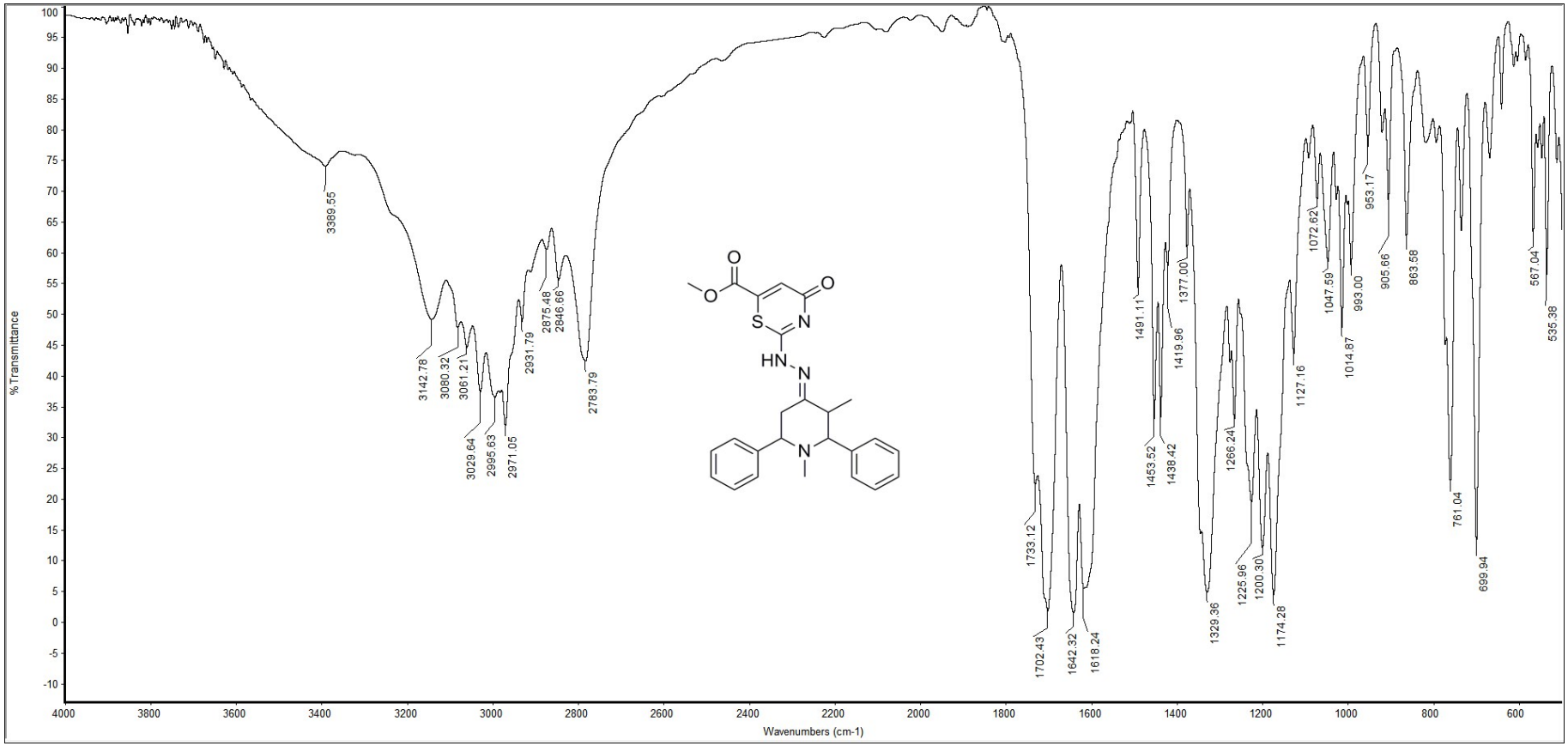


Fig. S 1 FT–IR Spectrum of compound **17**

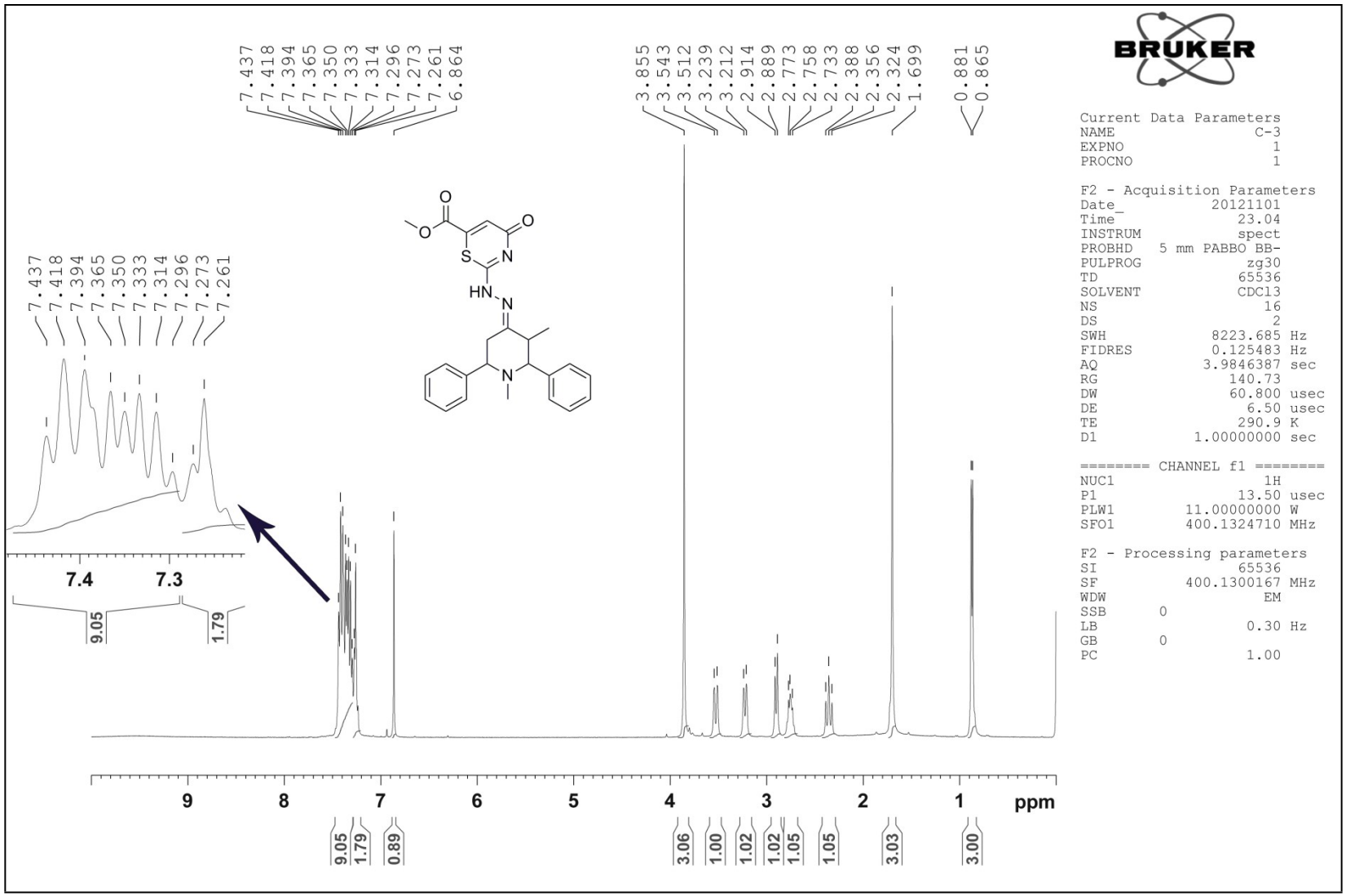


Fig. S 2 ^{1}H NMR Spectrum of Compound **17**

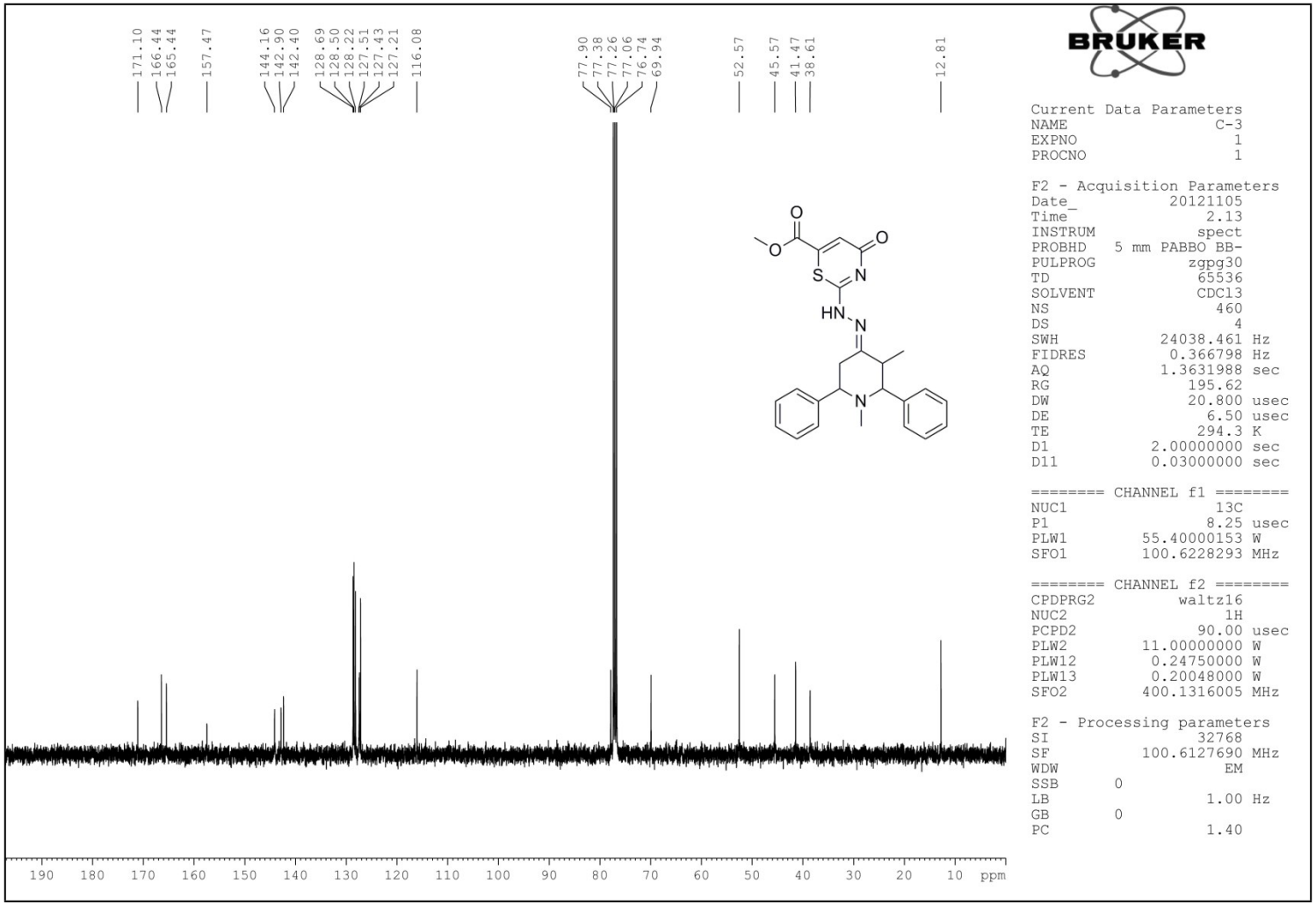
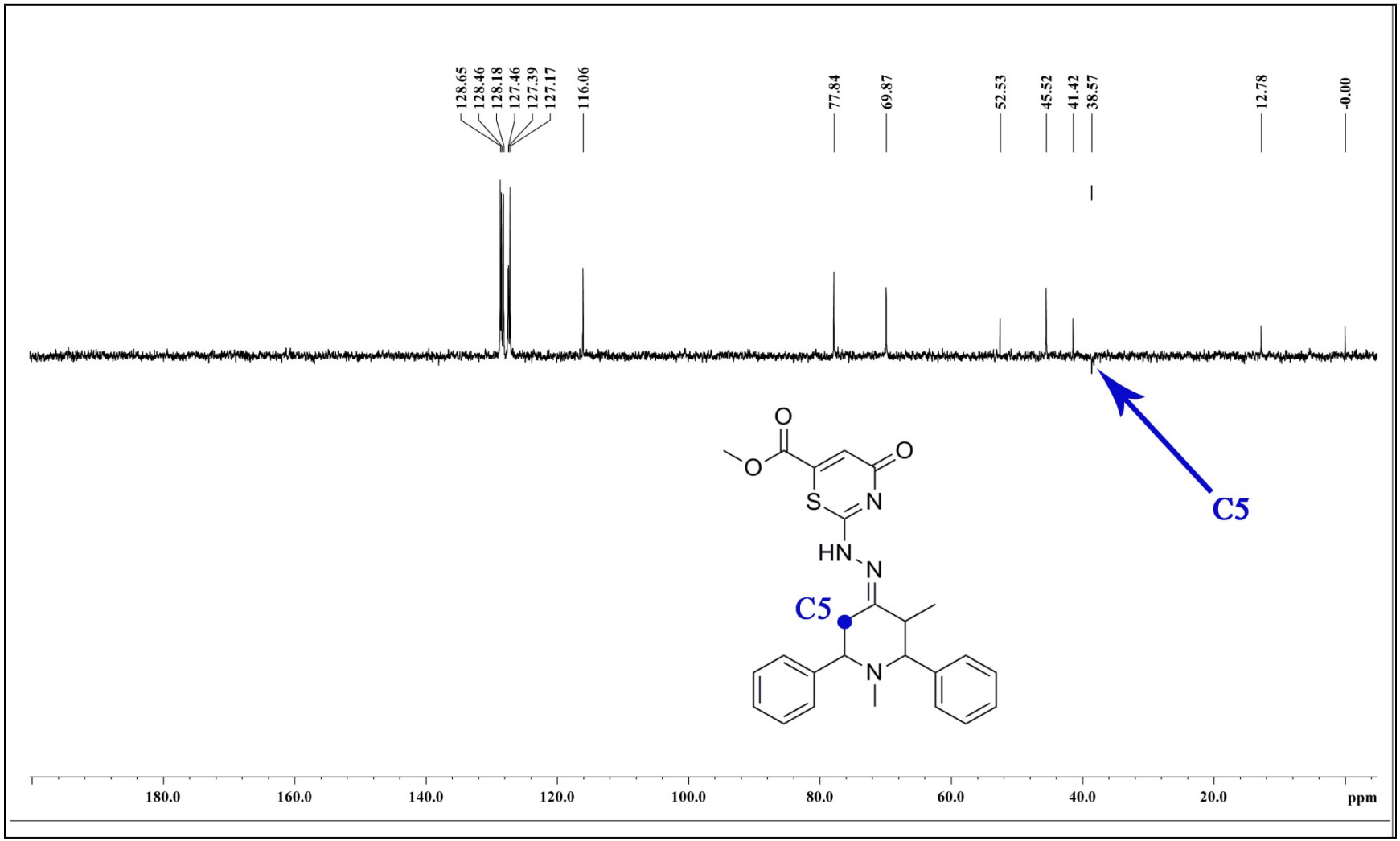


Fig. S 3 ^{13}C NMR spectrum of compound **17**



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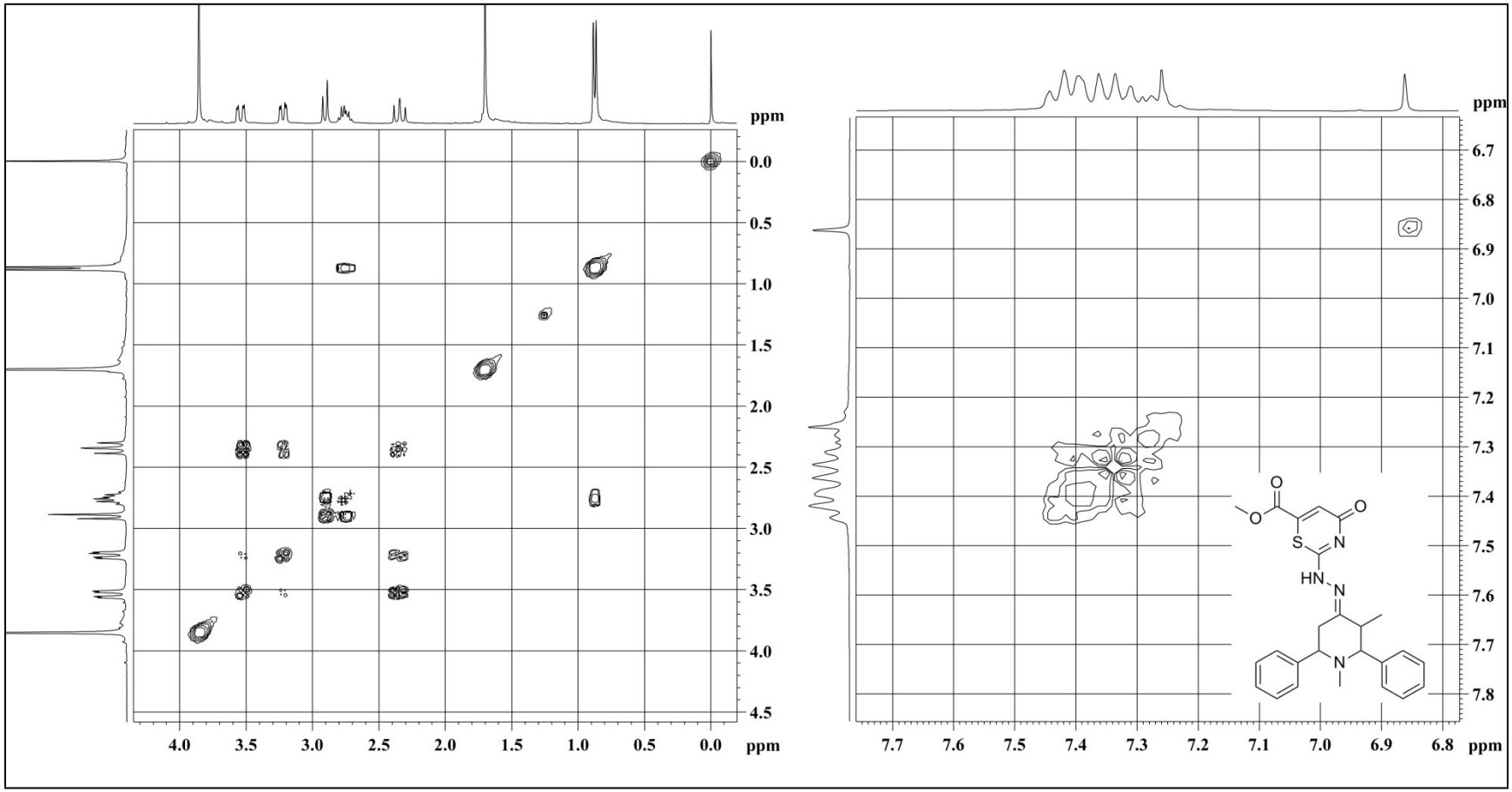


Fig. S 5 ^{1}H–^{1}H COSY NMR spectrum of compound **17**

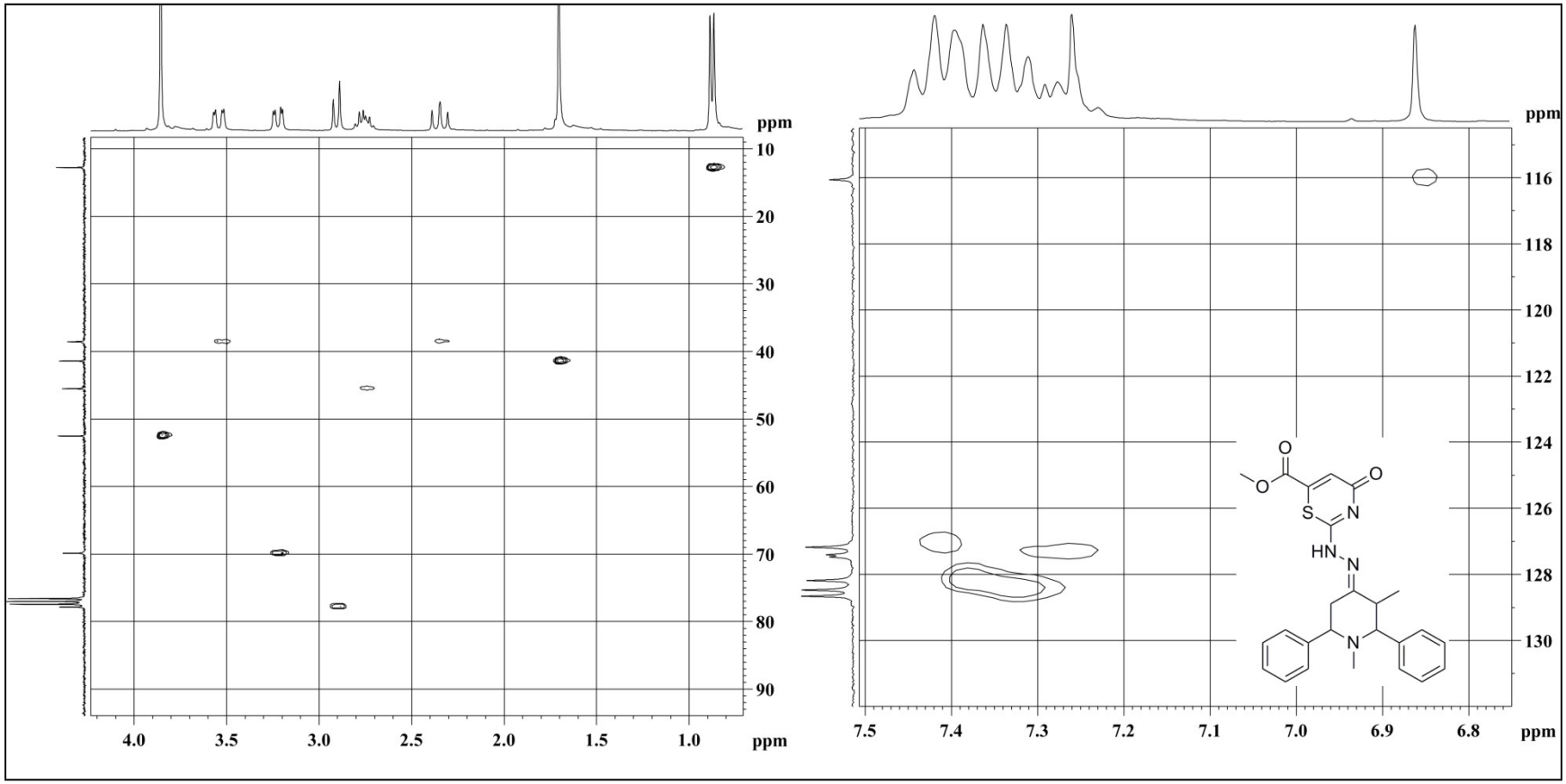


Fig. S 6 $^{1}H–^{13}C$ COSY NMR spectrum of compound **17**

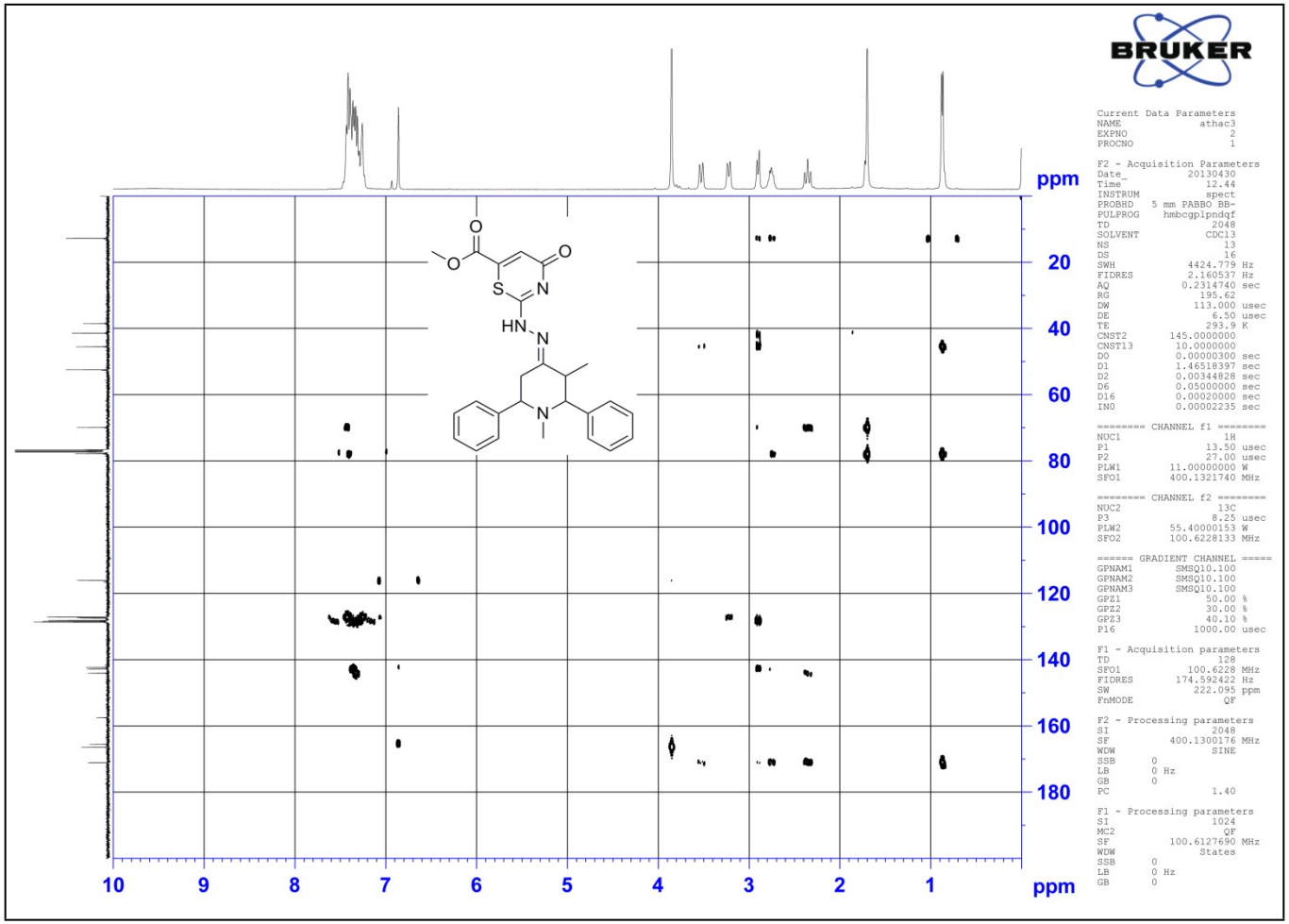
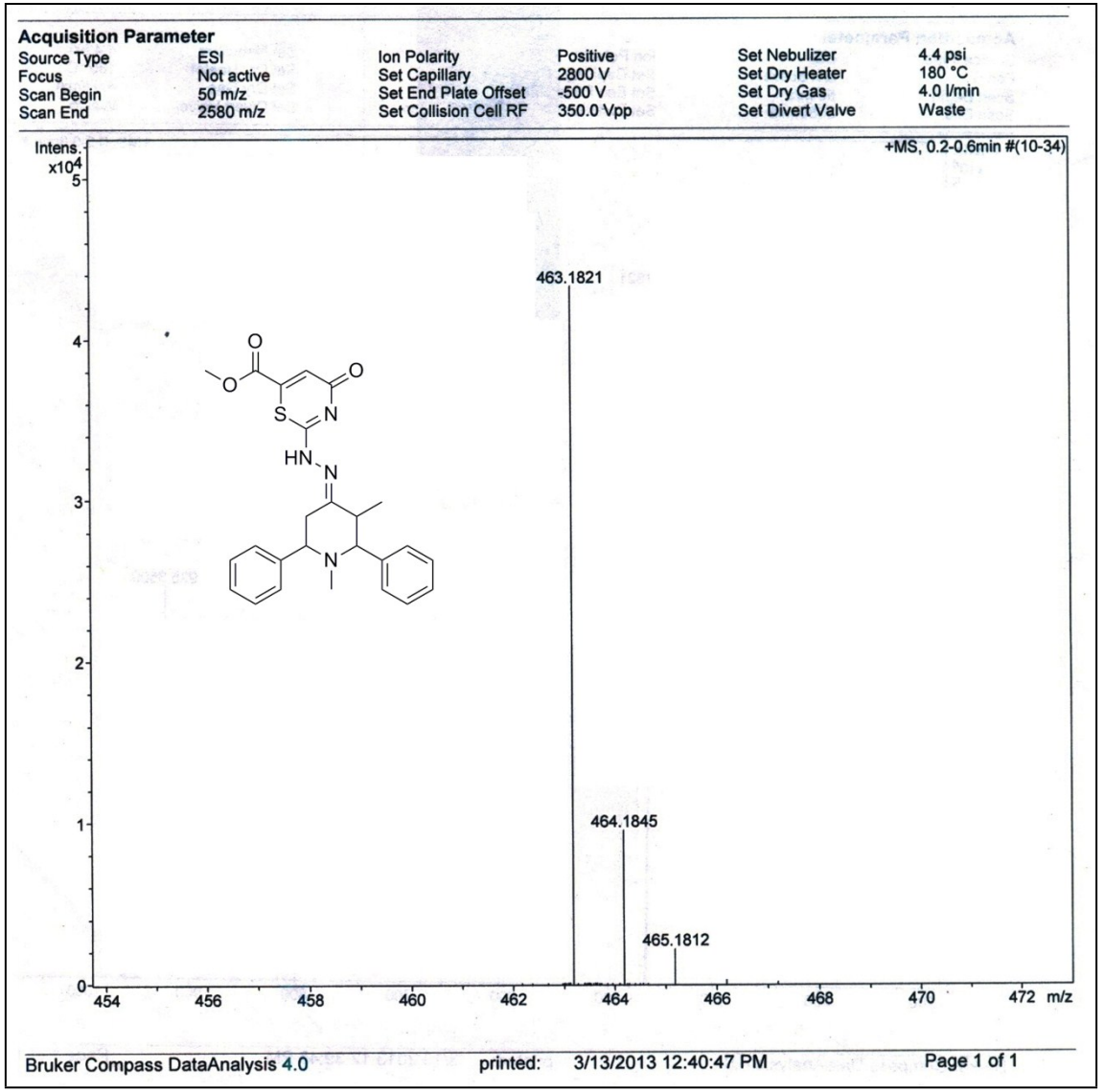


Fig. S 7 HMBC spectrum of compound **17**



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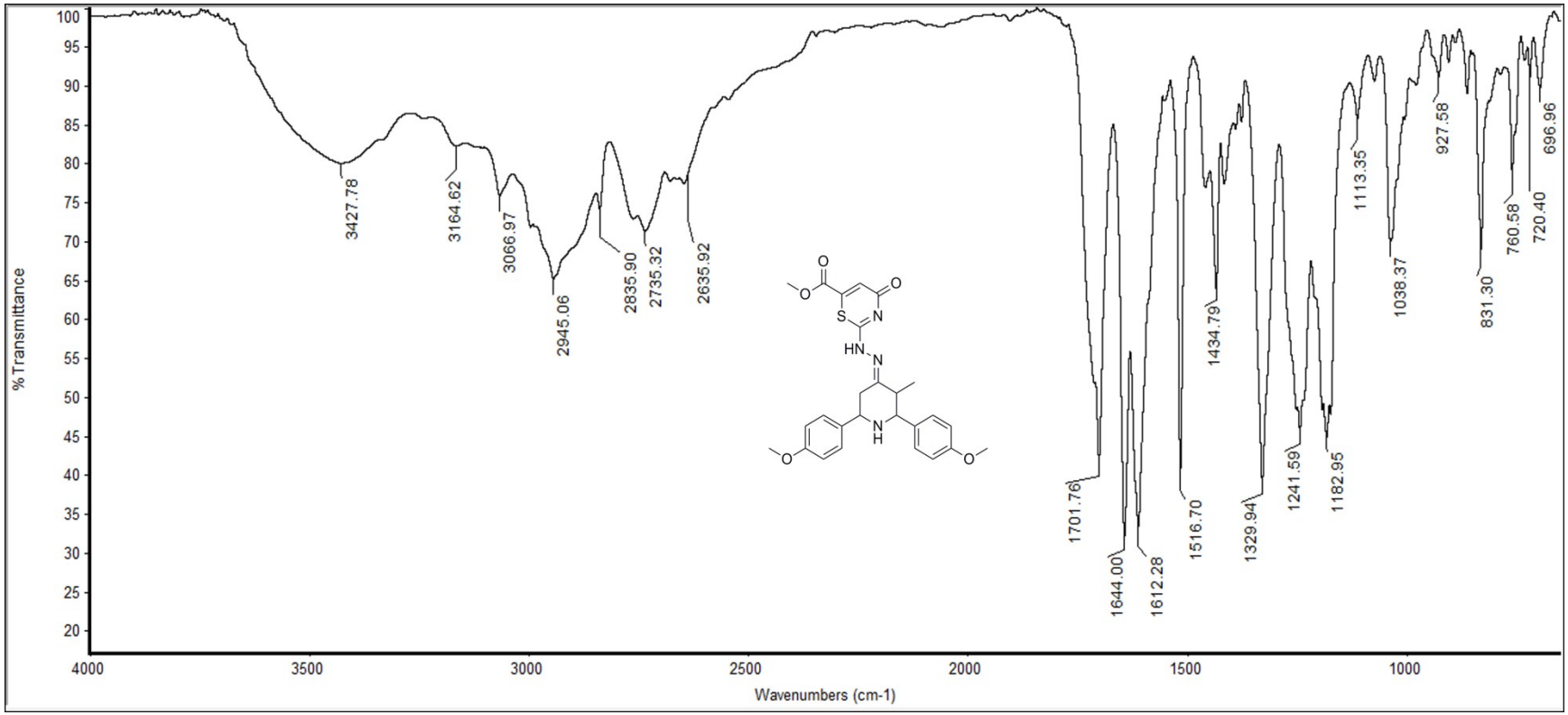


Fig. S 9 FT–IR spectrum of compound **18**

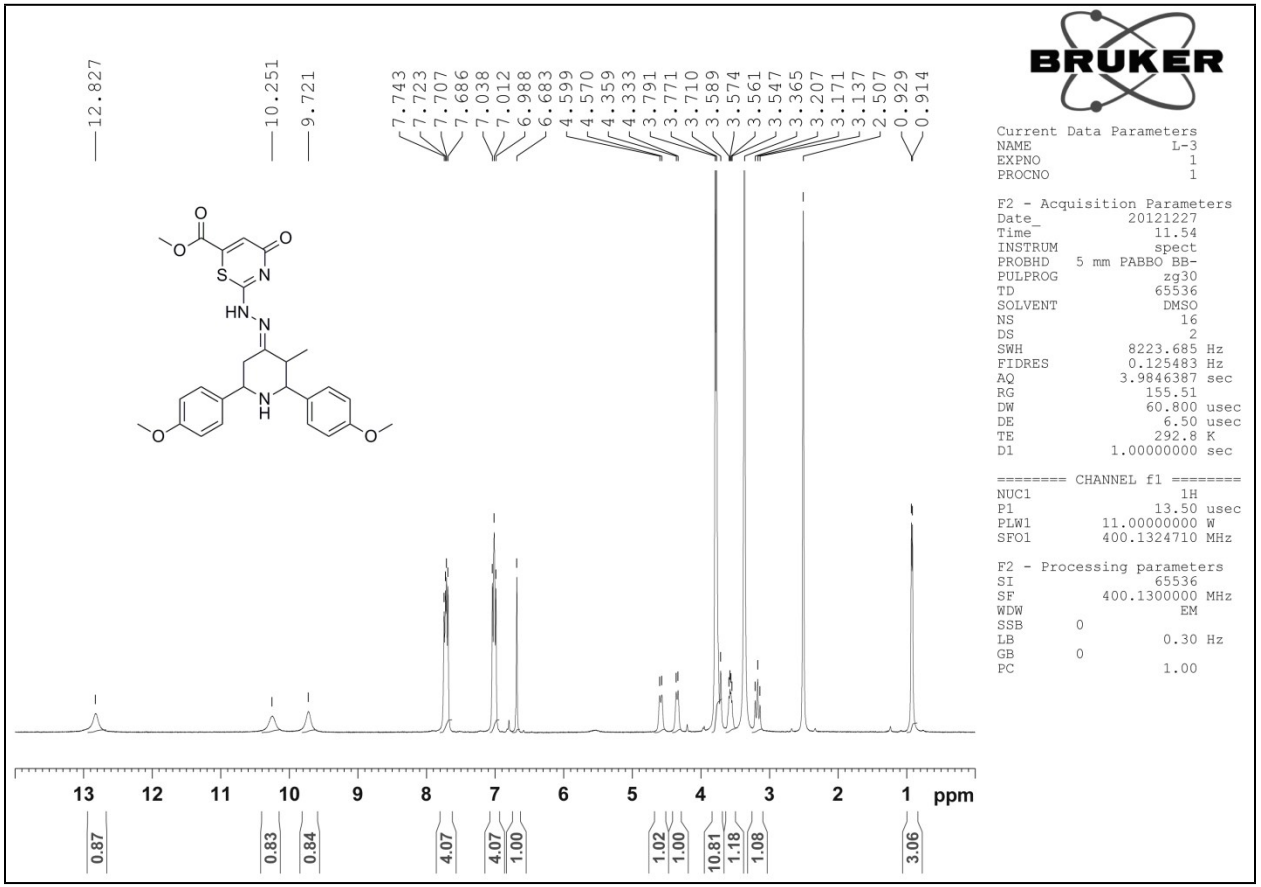
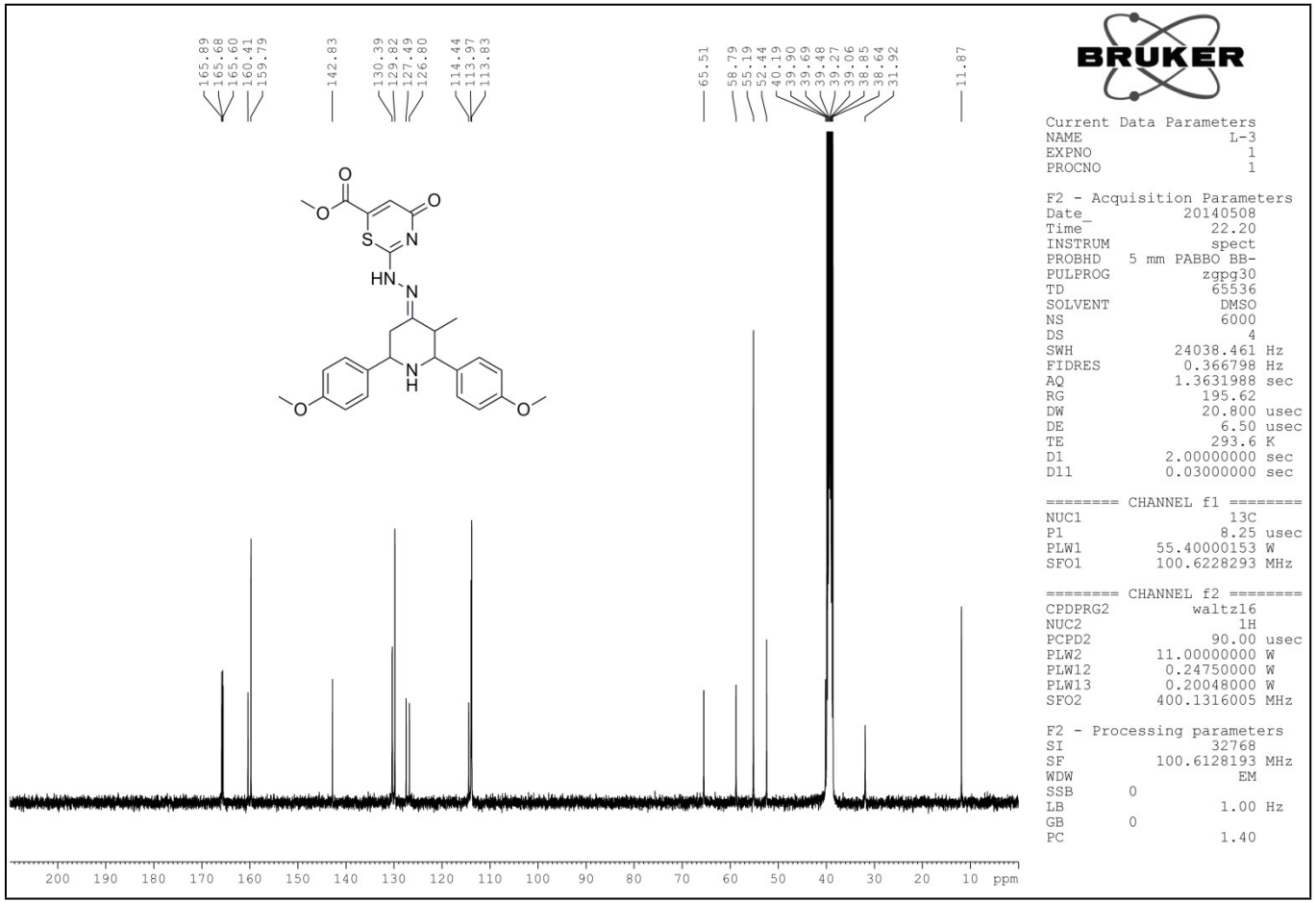


Fig. S 10 ^{1}H NMR Spectrum of Compound **18**



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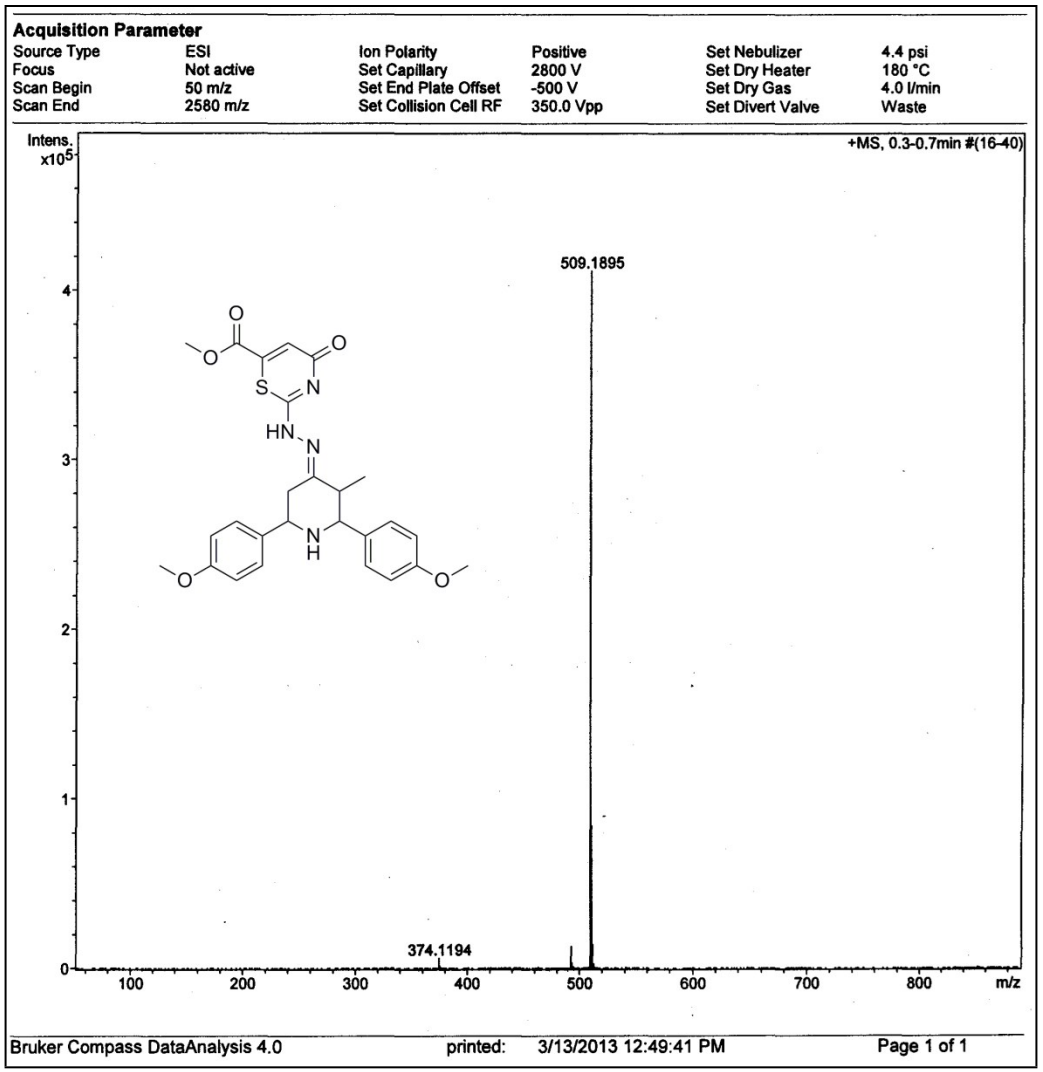


Fig. S 12 HR–Mass spectrum of compound **18**

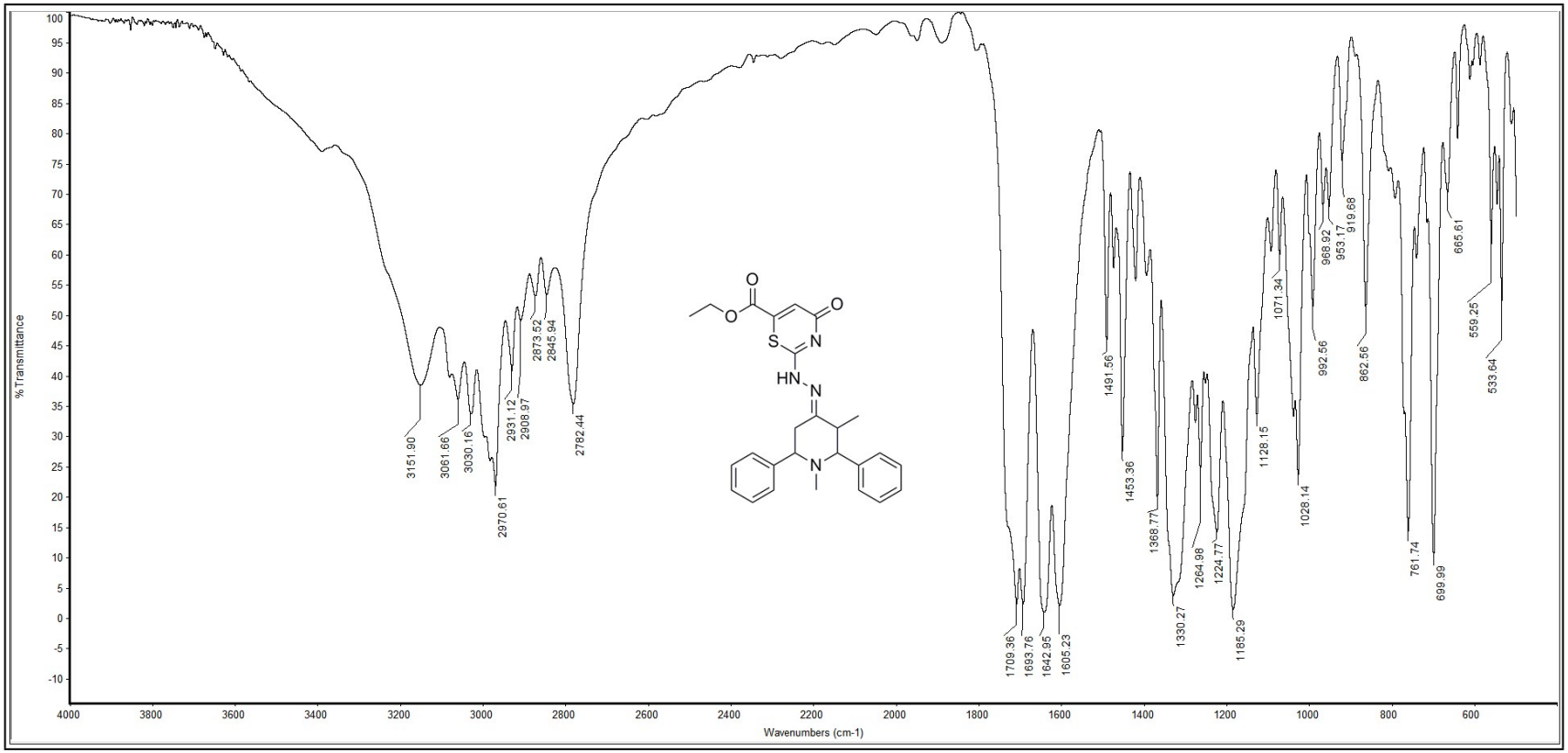


Fig. S 13 FT–IR spectrum of compound **19**

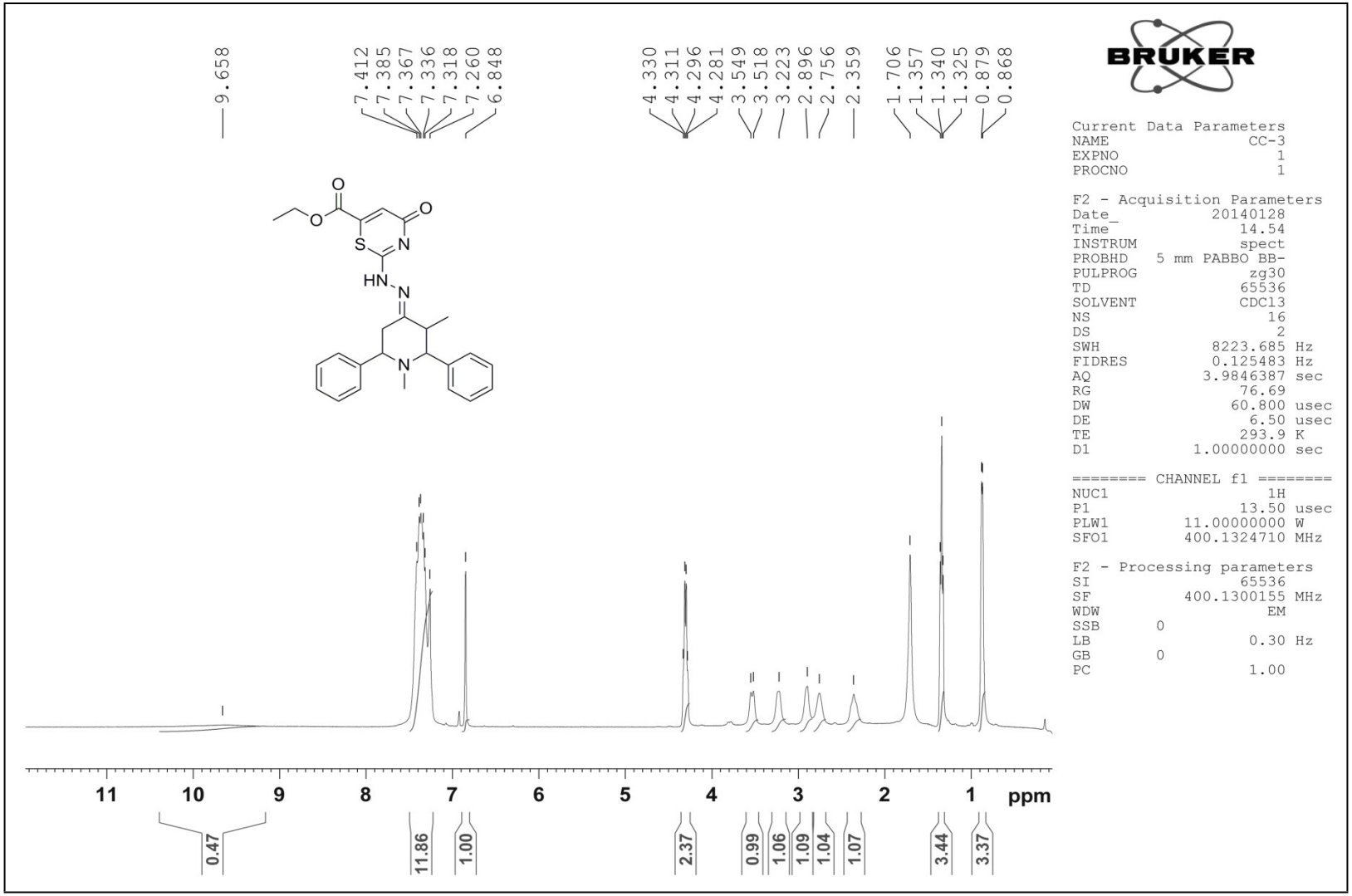


Fig. S 14 ^{1}H NMR Spectrum of Compound **19**

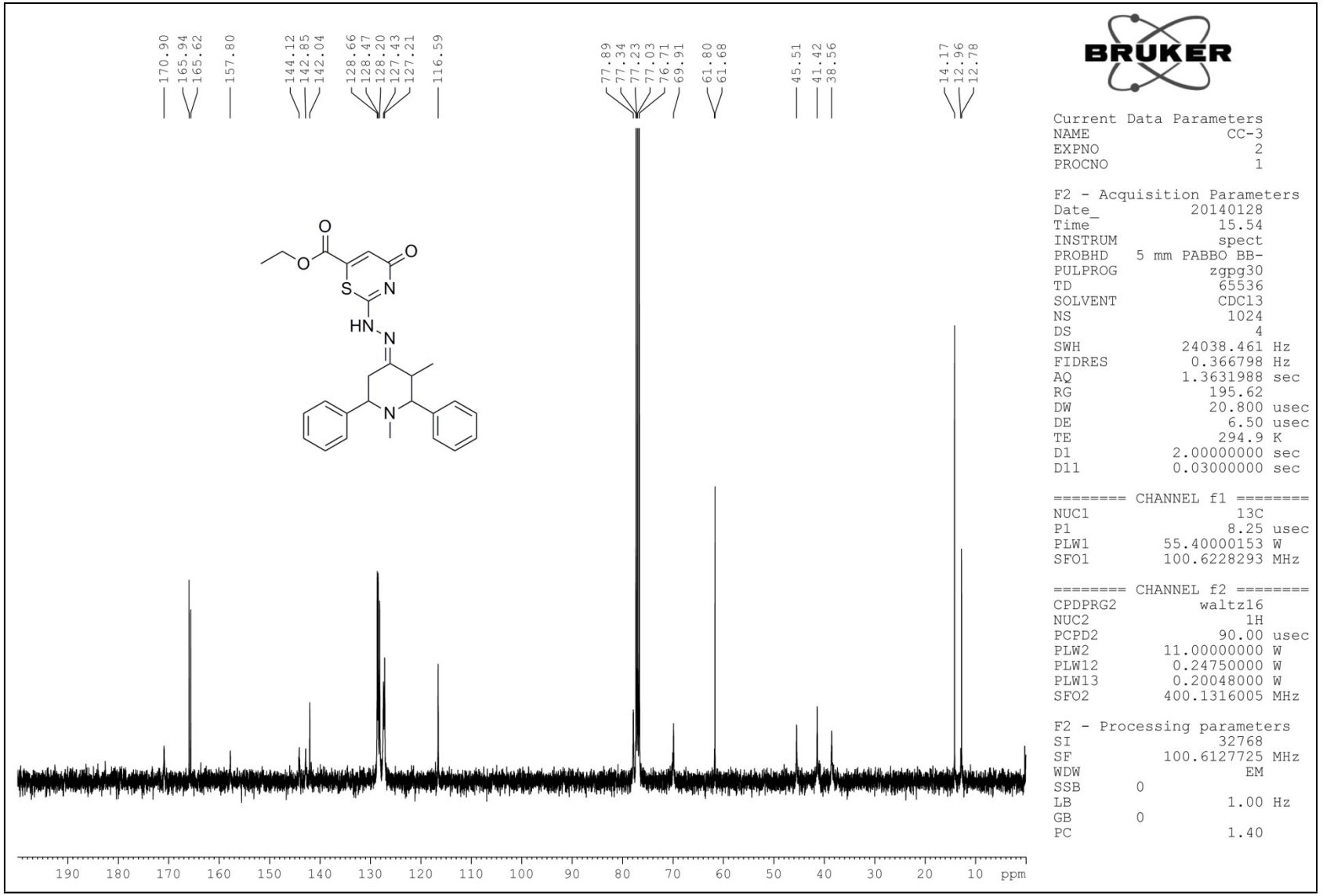


Fig. S 15 ^{13}C NMR spectrum of compound **19**

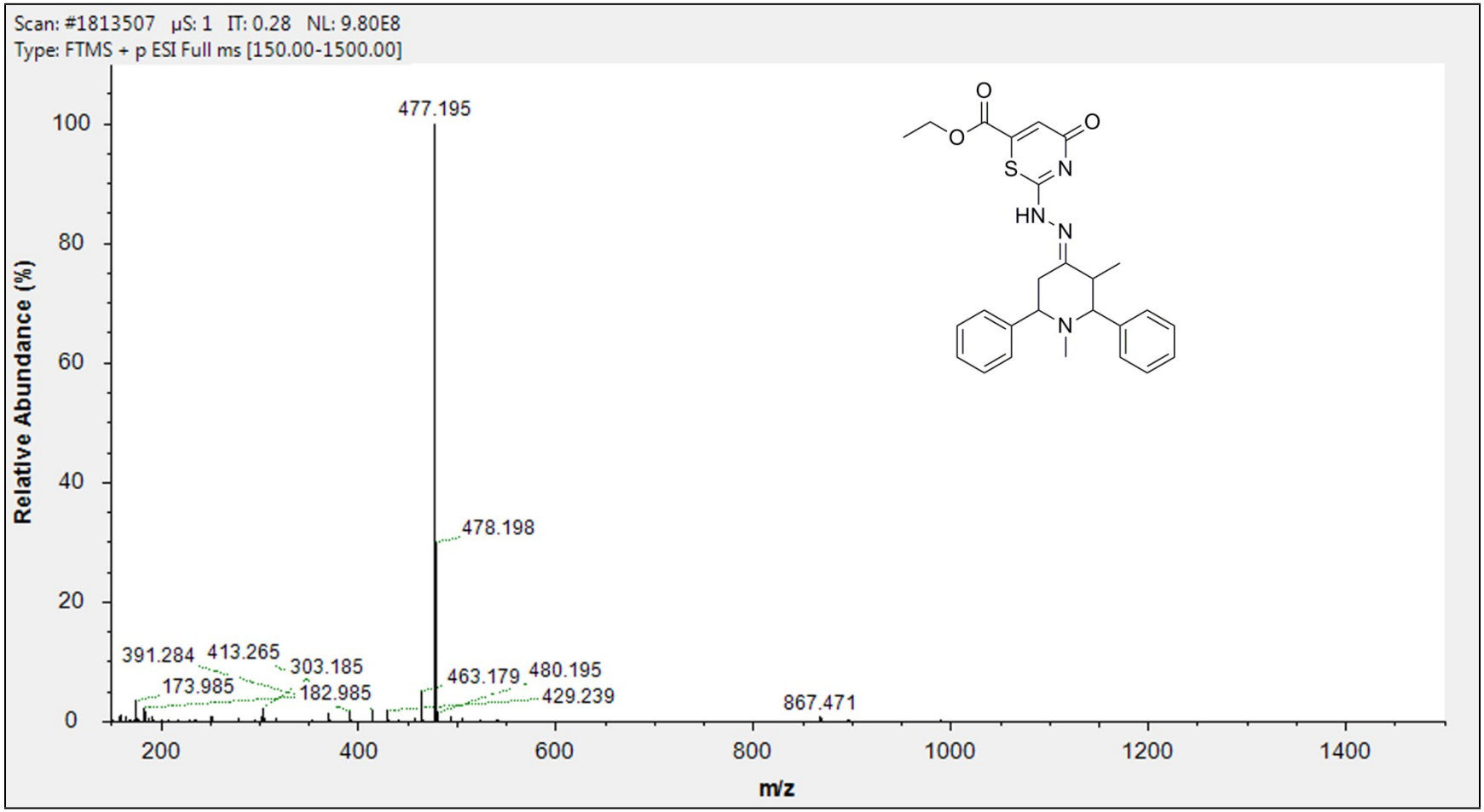


Fig. S 16 Mass spectrum of compound **19**

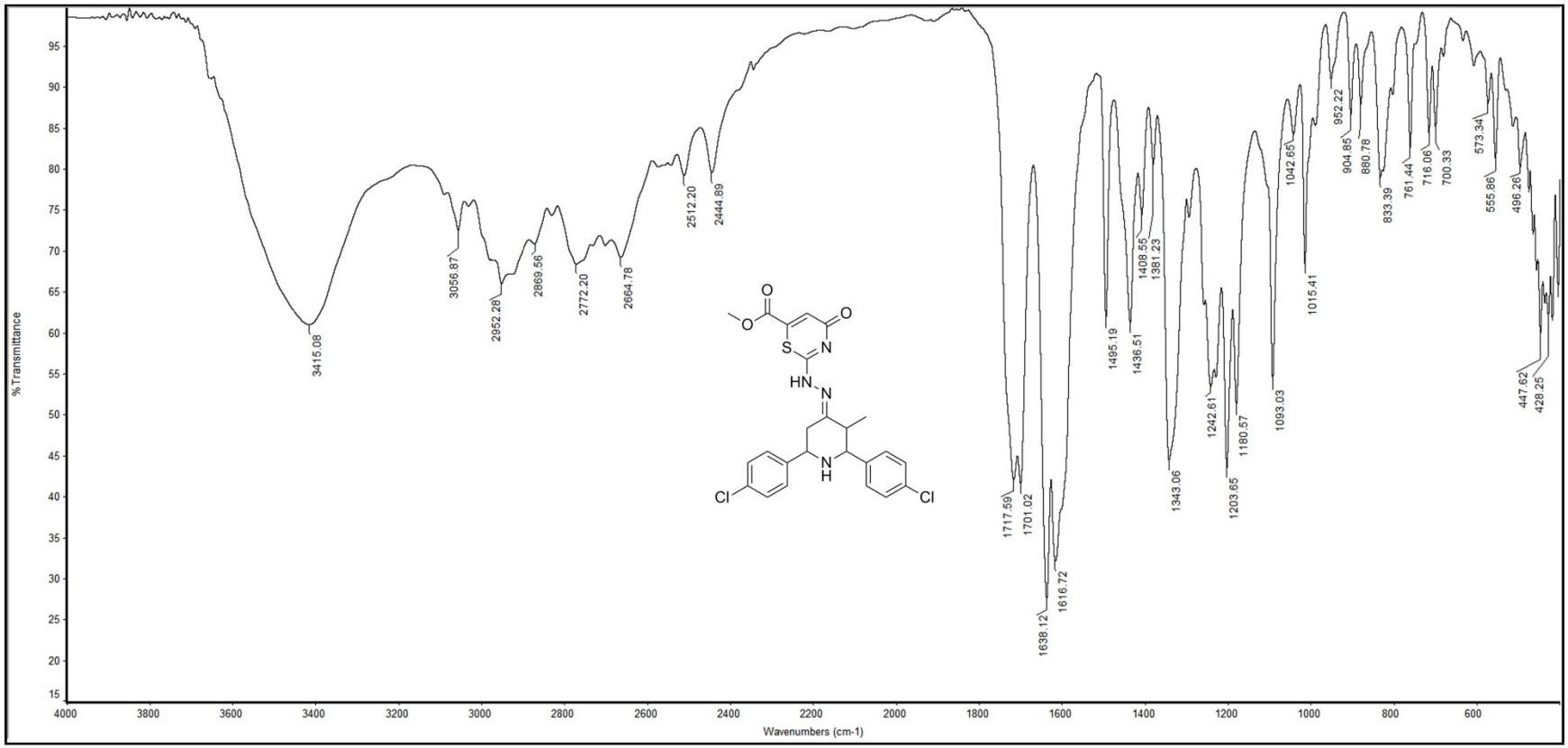


Fig. S 17 FT–IR spectrum of compound **20**

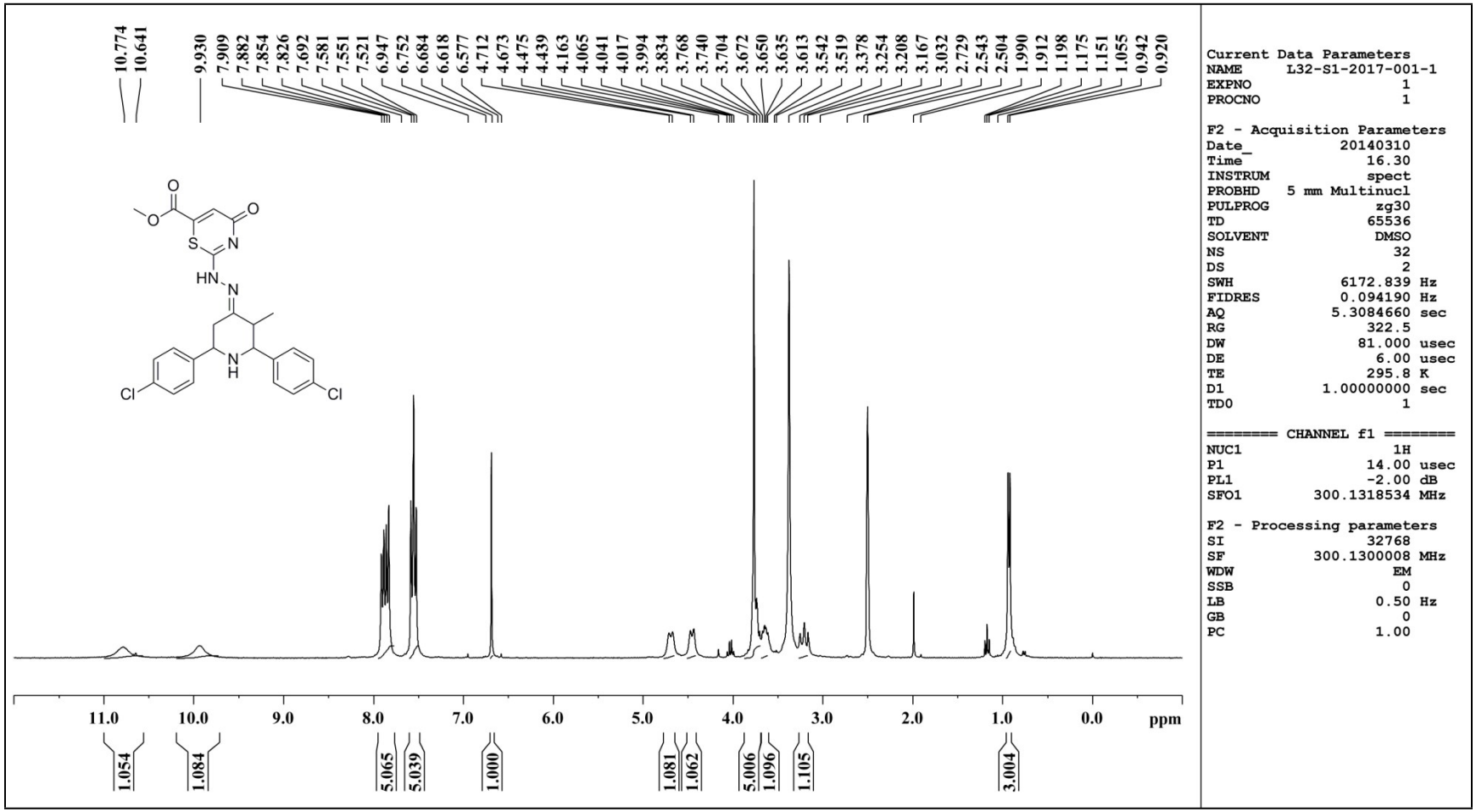


Fig. S 18 ^{1}H NMR Spectrum of Compound **20**

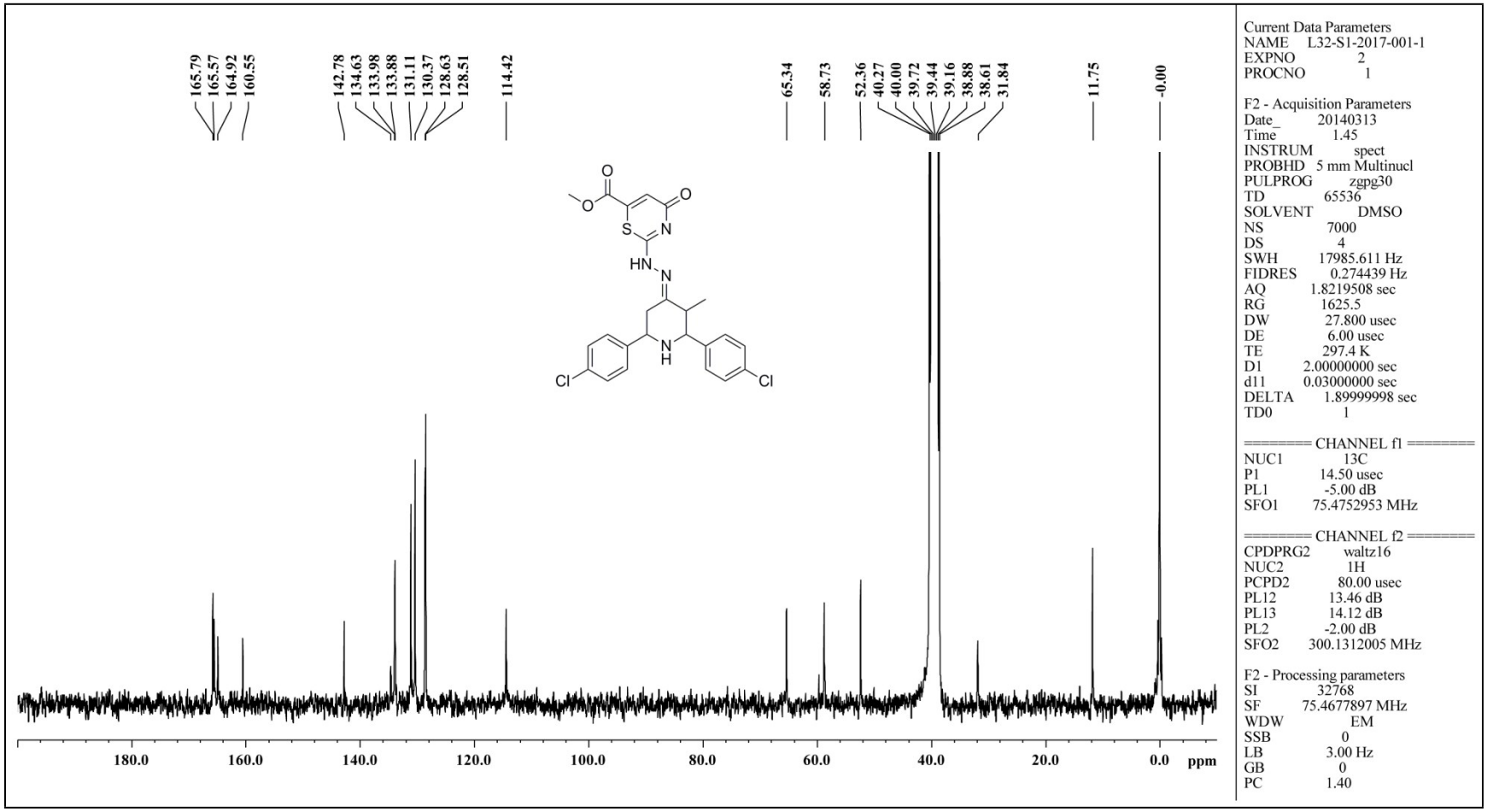


Fig. S 19 ^{13}C NMR spectrum of compound **20**

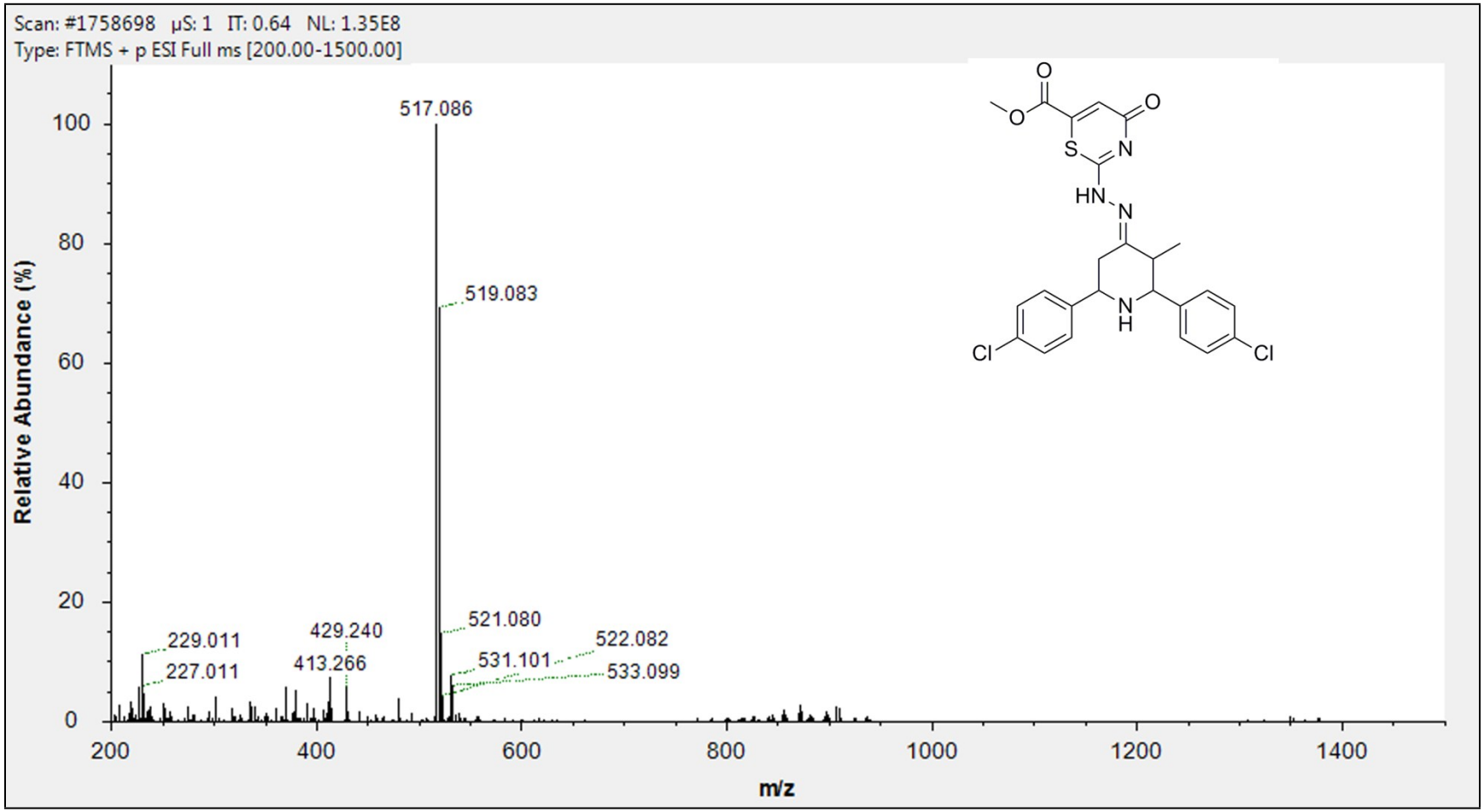


Fig. S 20 Mass spectrum of compound **20**

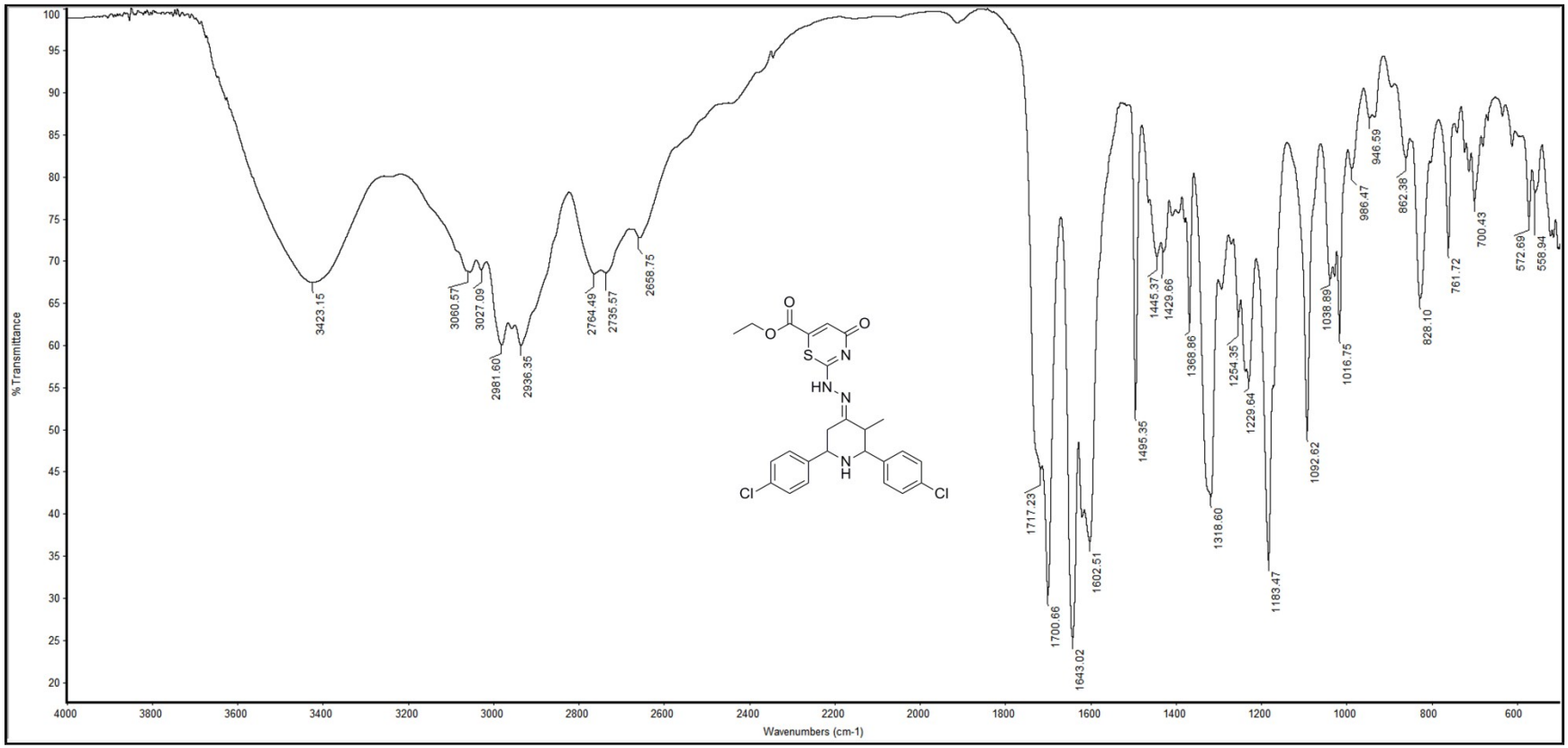


Fig. S 21 FT–IR spectrum of compound **21**

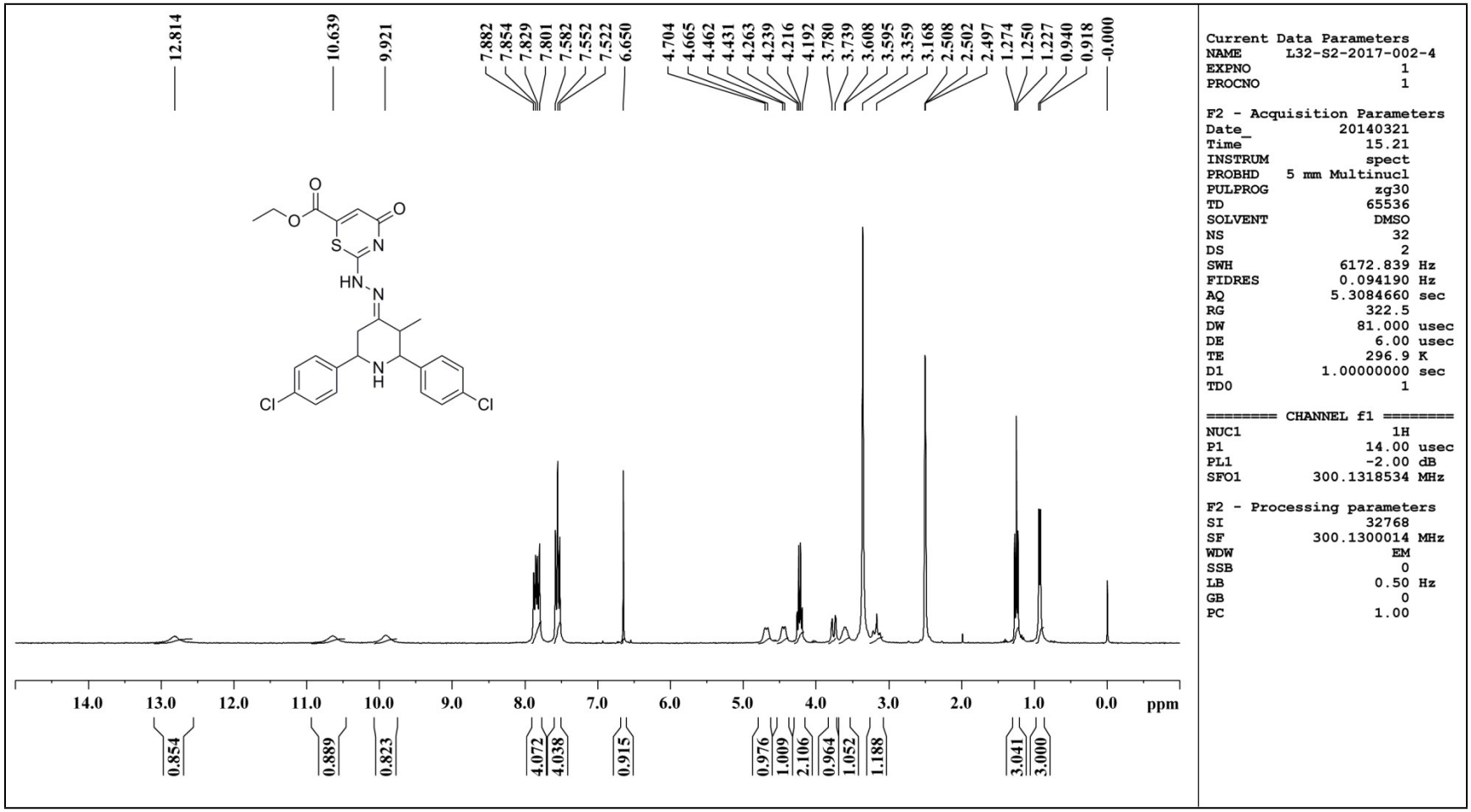


Fig. S 22 ^{1}H NMR Spectrum of Compound **21**

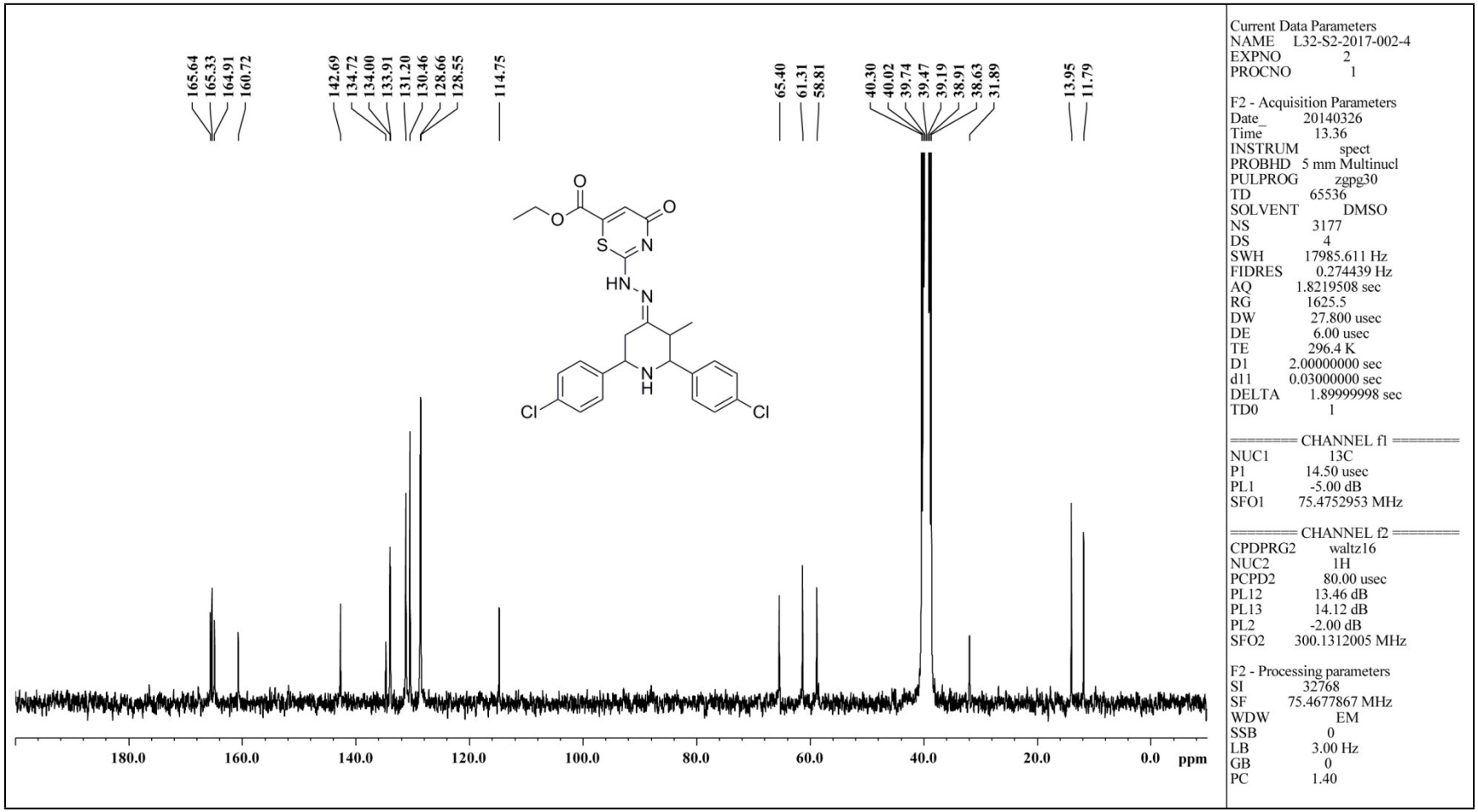


Fig. S 23 ^{13}C NMR spectrum of compound **21**

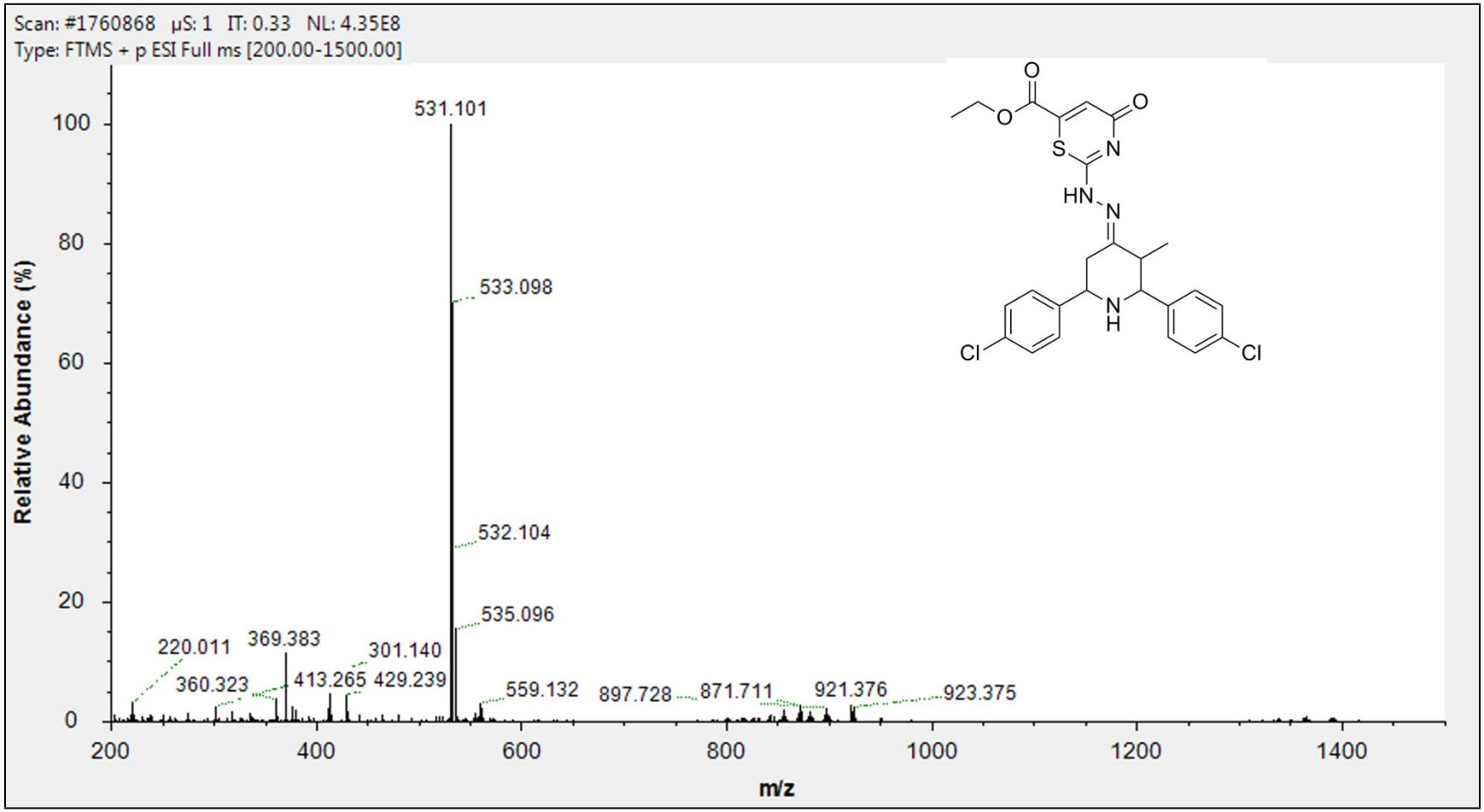


Fig. S 24 Mass spectrum of compound **21**

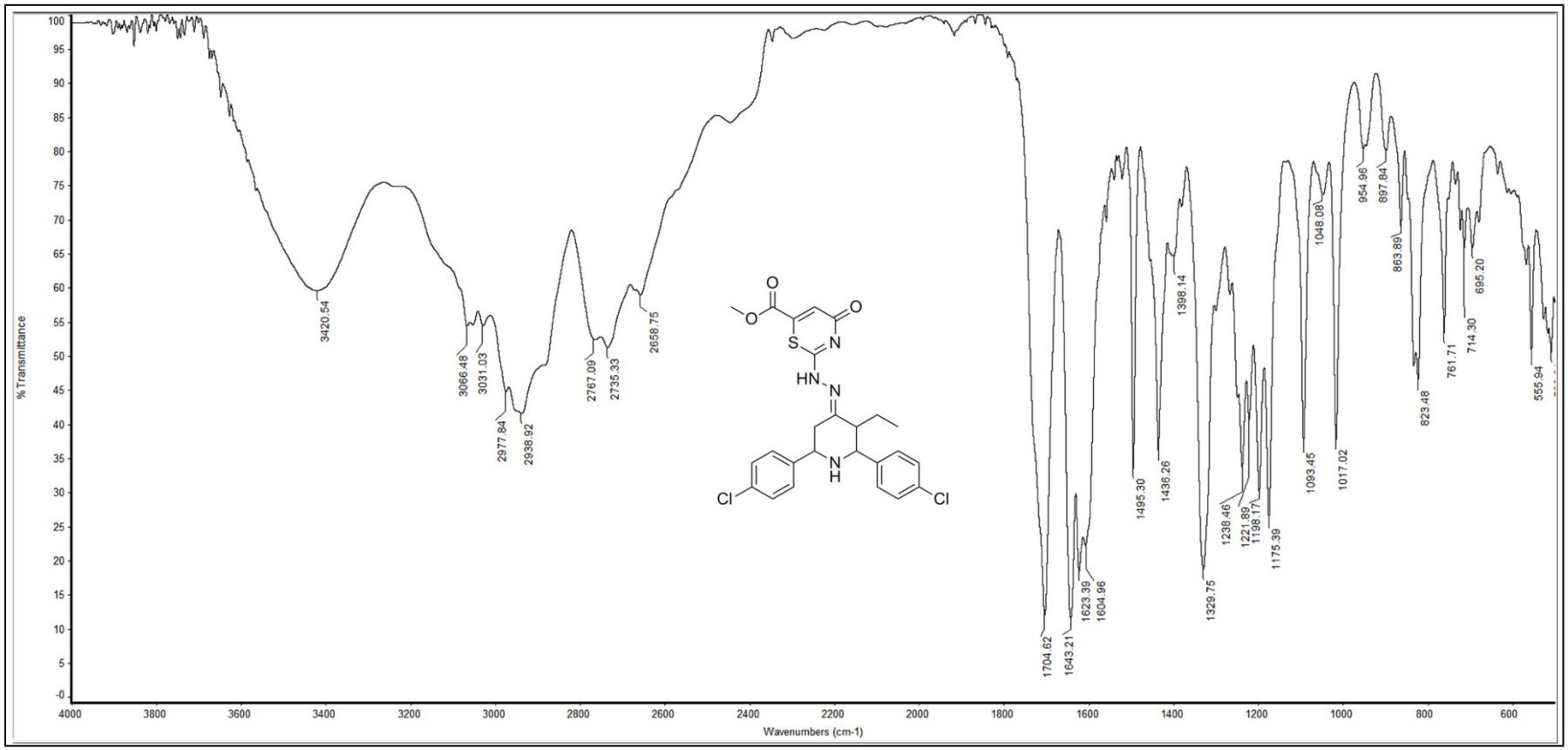


Fig. S 25 FT–IR spectrum of compound **22**

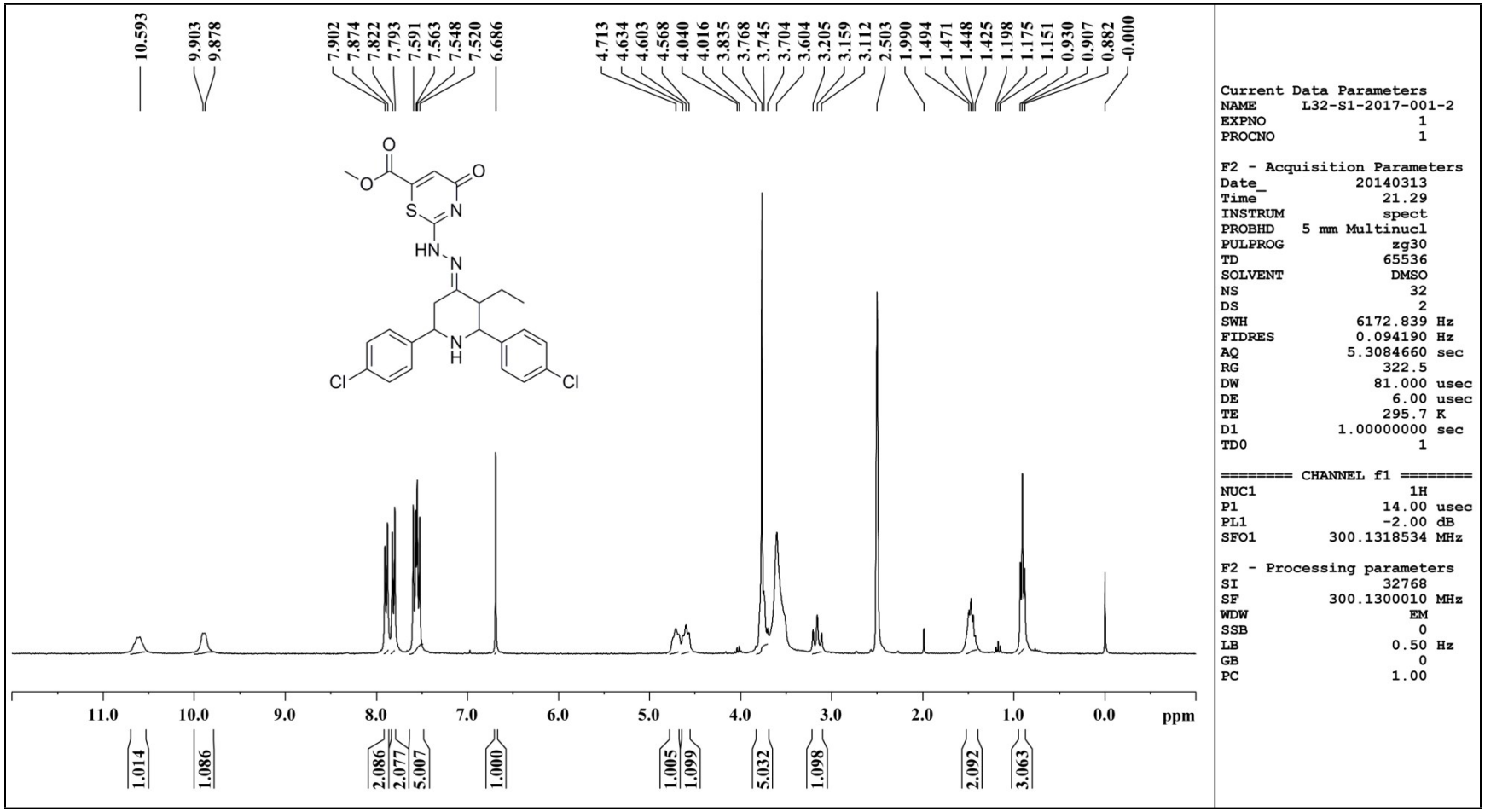


Fig. S 26 ^{1}H NMR Spectrum of compound **22**

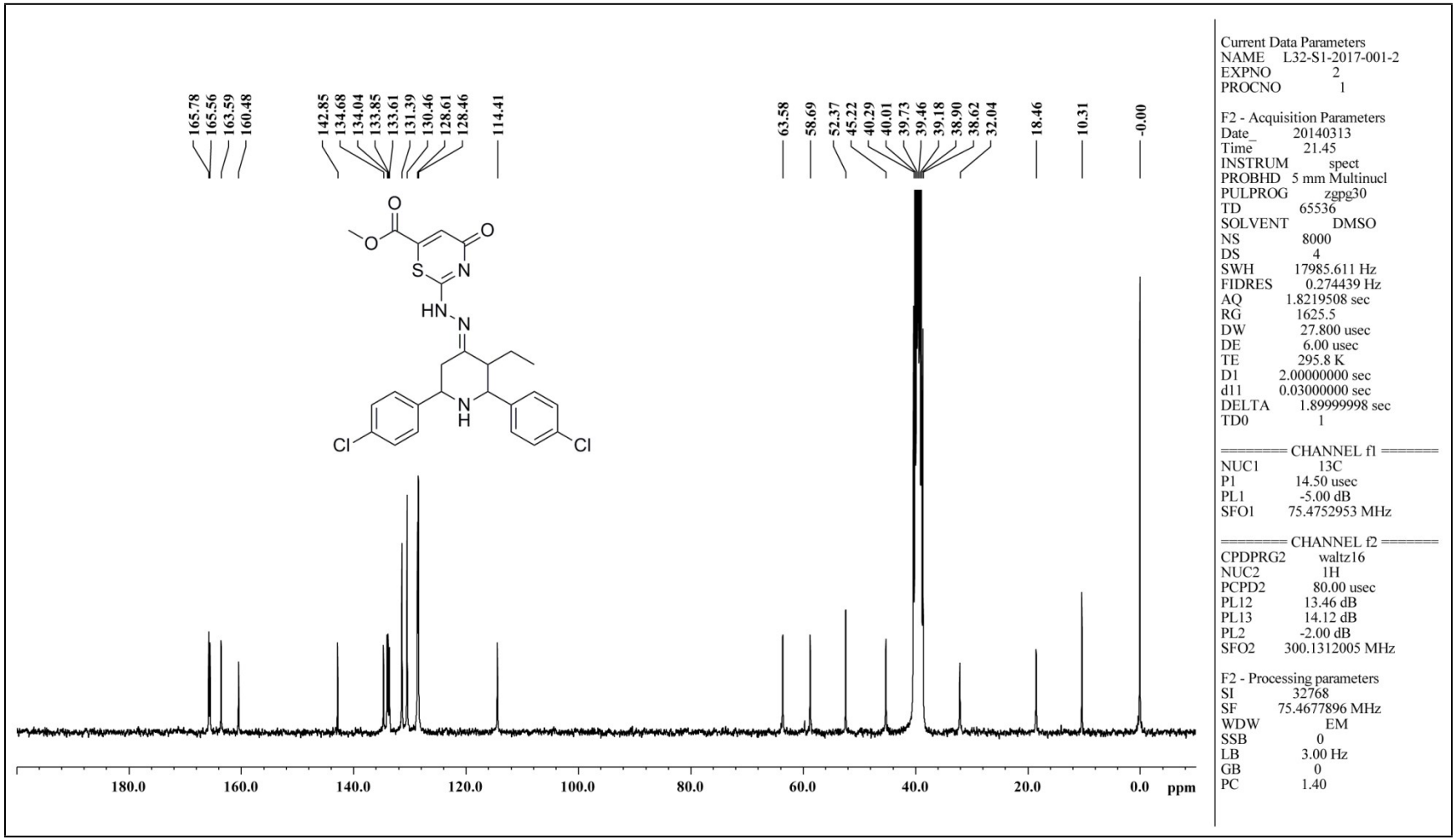


Fig. S 27 ^{13}C NMR spectrum of compound **22**

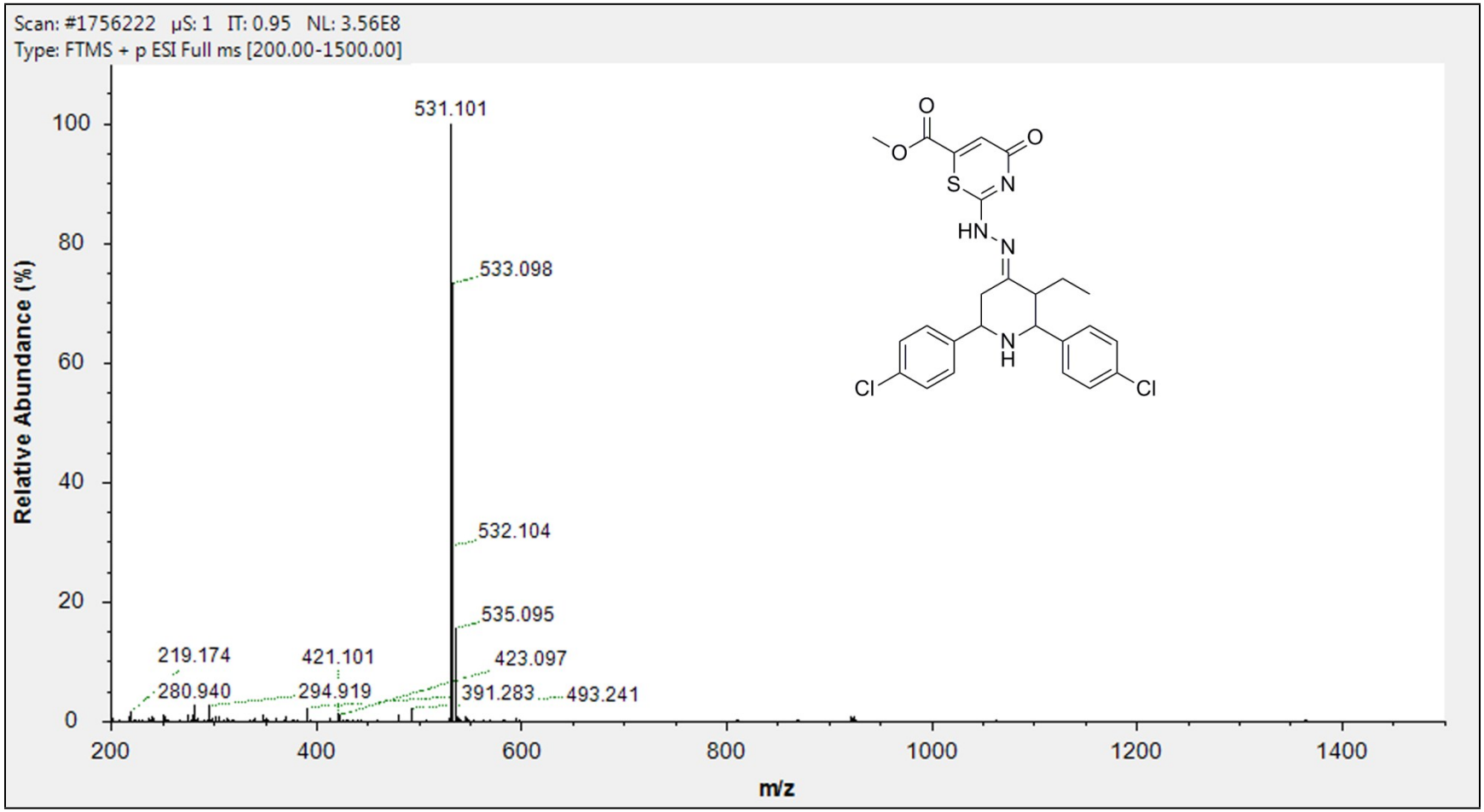


Fig. S 28 Mass spectrum of compound **22**

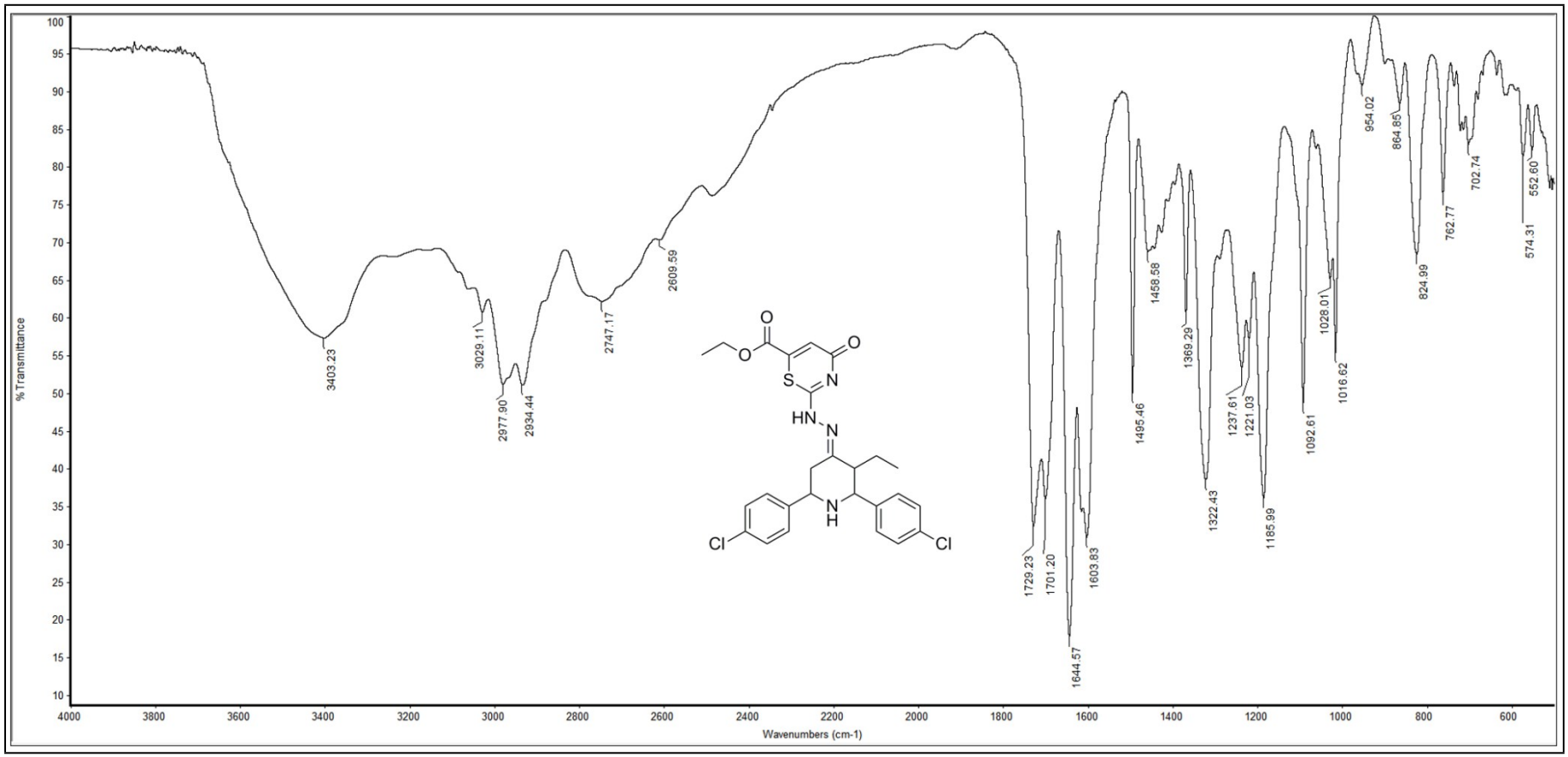


Fig. S 29 FT–IR spectrum of compound **23**

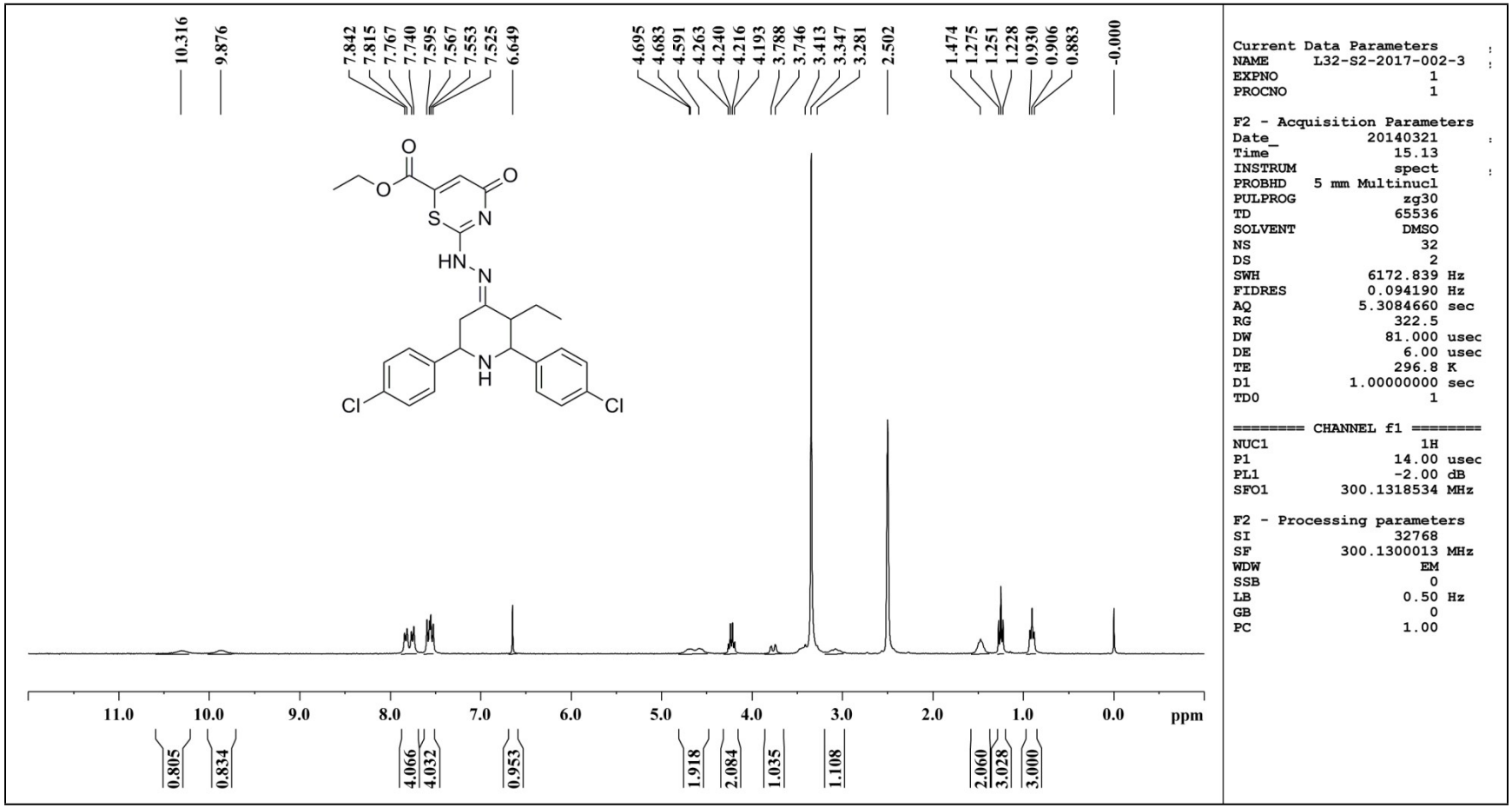


Fig. S 30 ^{1}H NMR Spectrum of compound **23**

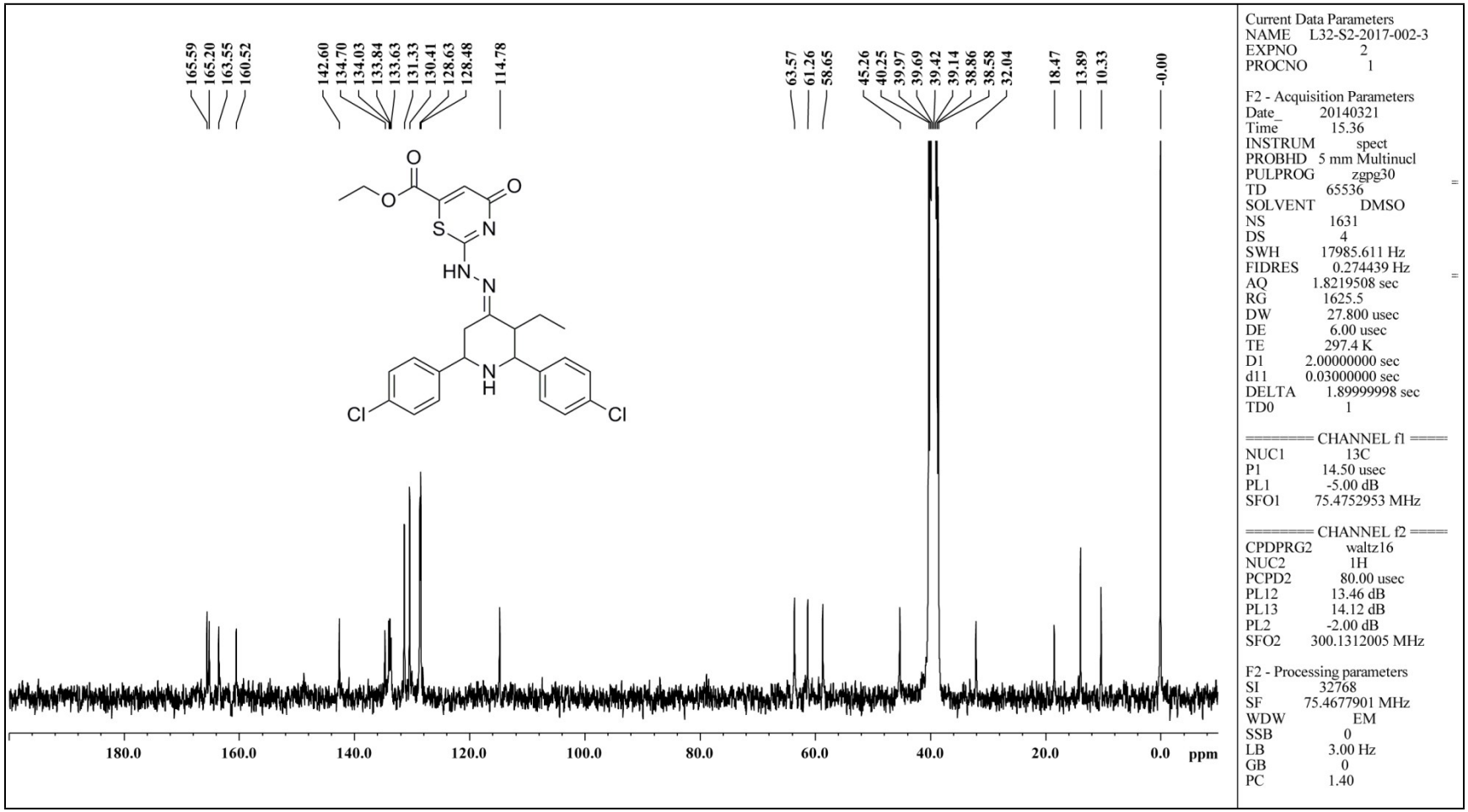


Fig. S 31 ^{13}C NMR spectrum of compound **23**

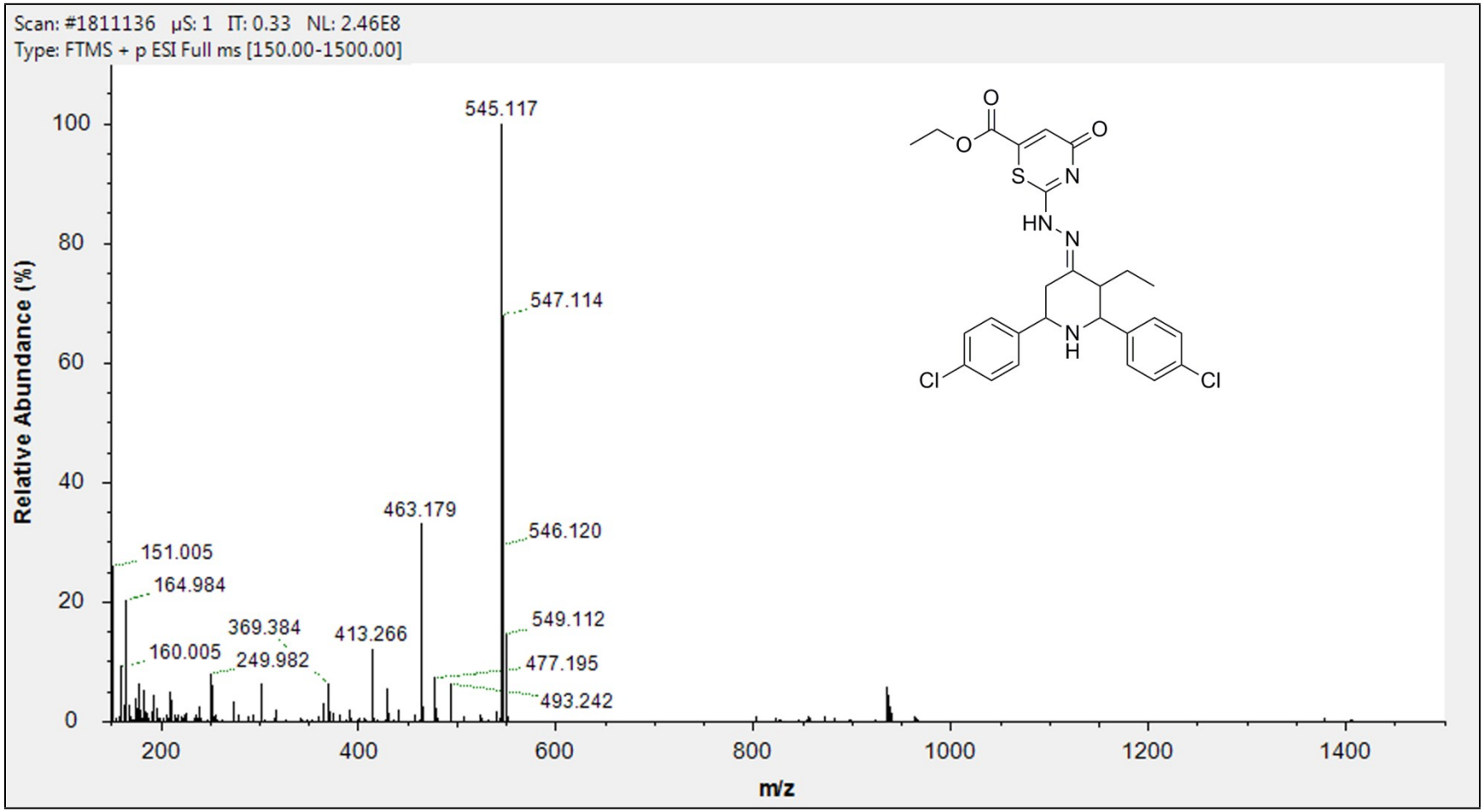


Fig. S 32 Mass spectrum of compound **23**

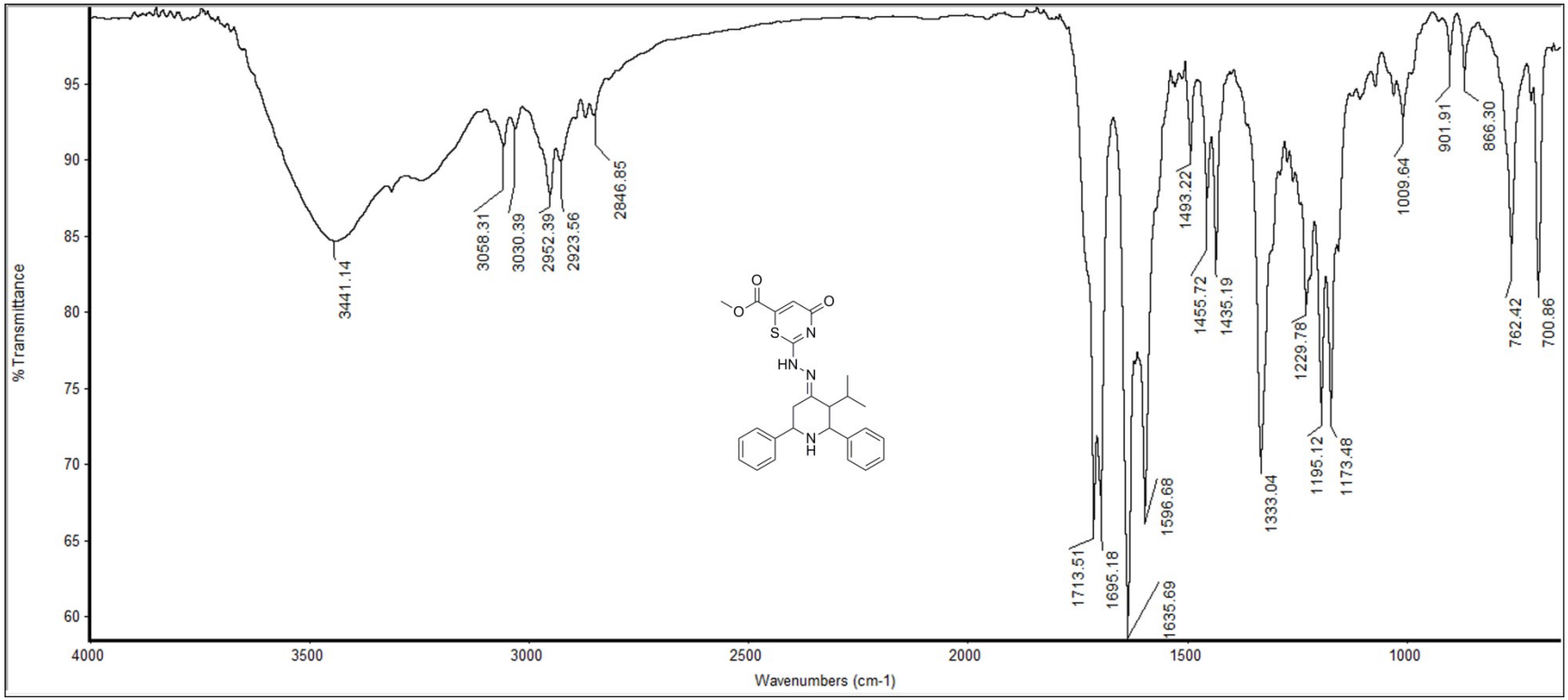


Fig. S 33 FT–IR spectrum of compound **24**

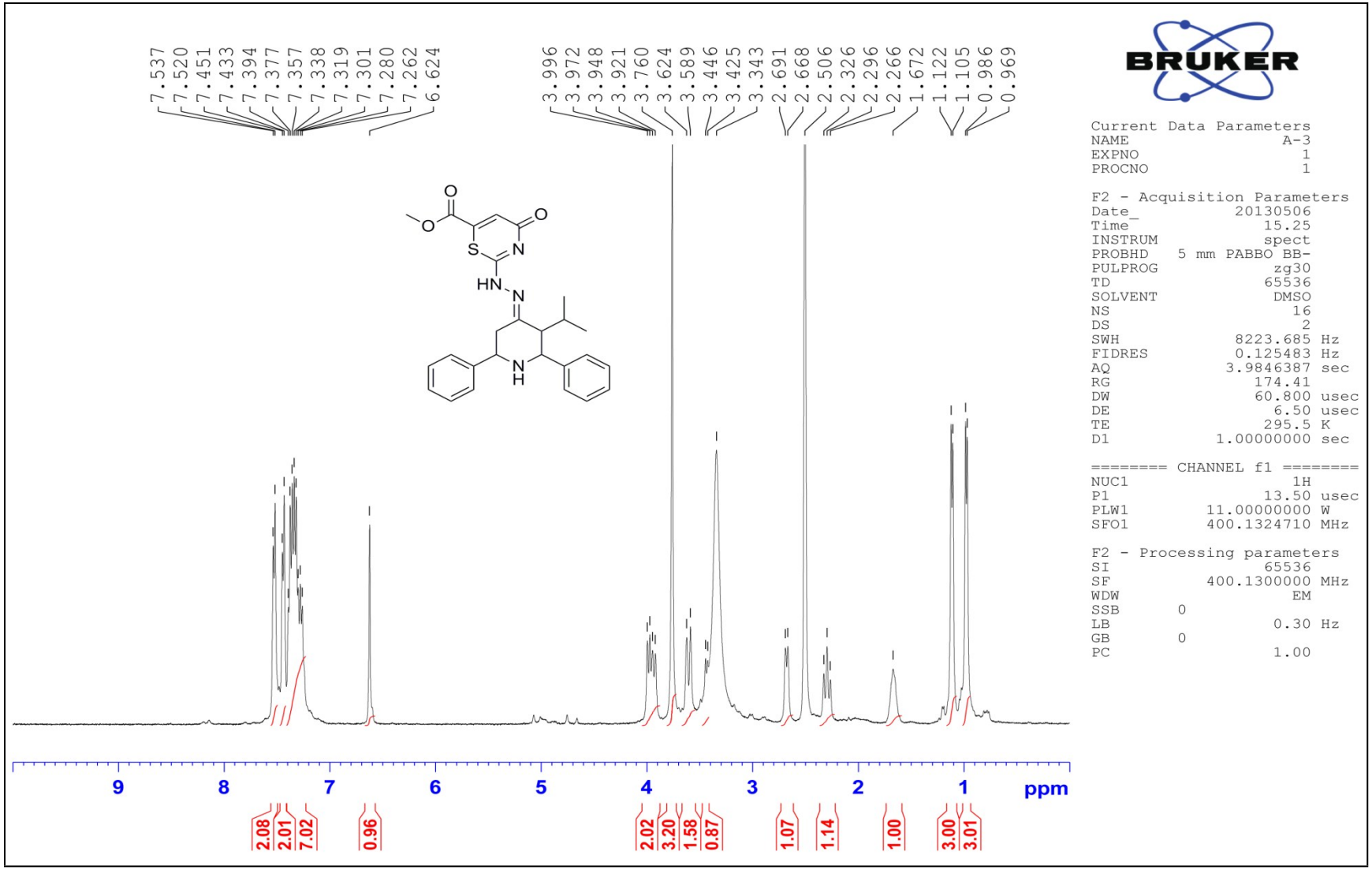


Fig. S 34 ^{1}H NMR Spectrum of Compound **24**

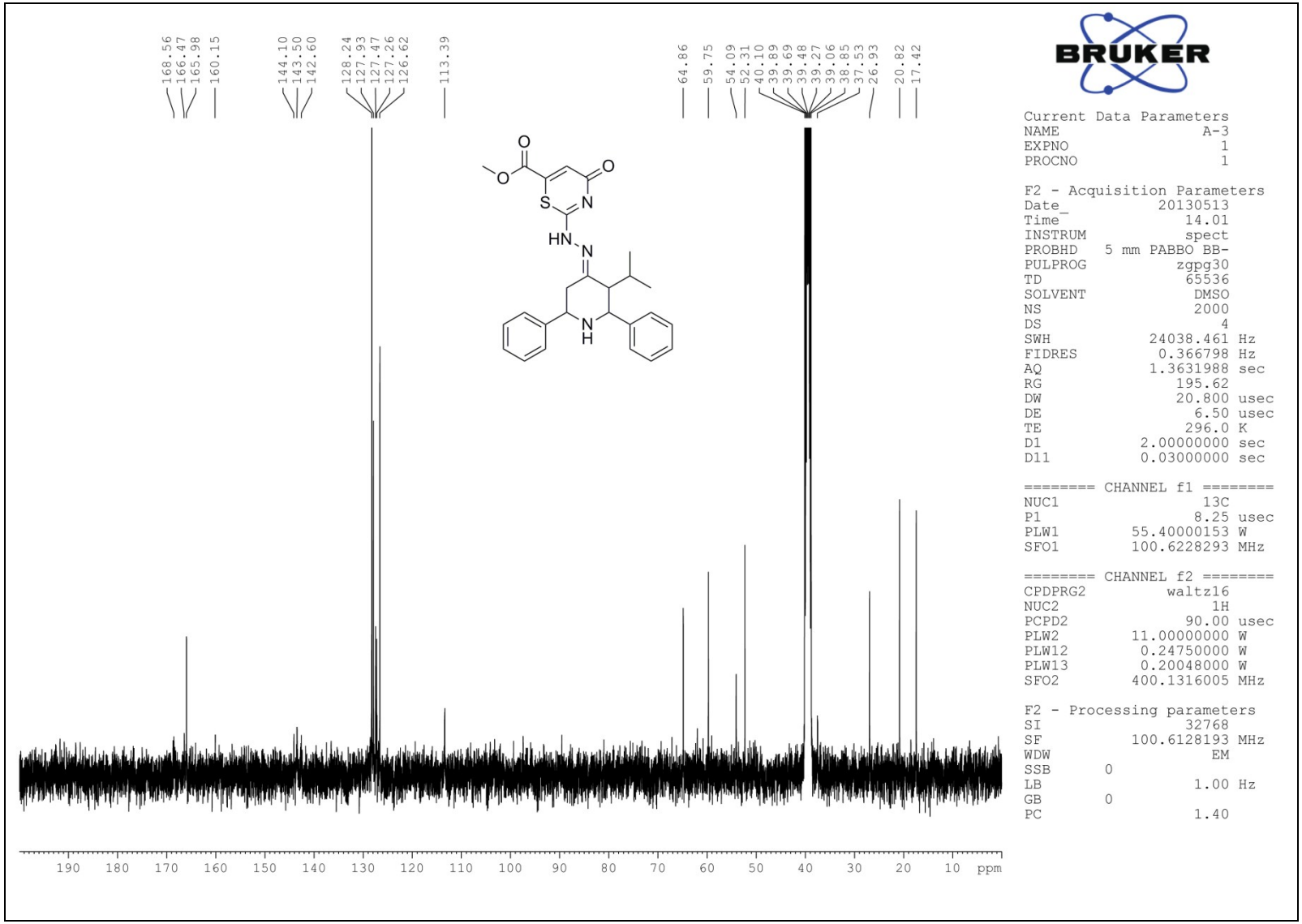


Fig. S 35 ^{13}C NMR spectrum of compound **24**

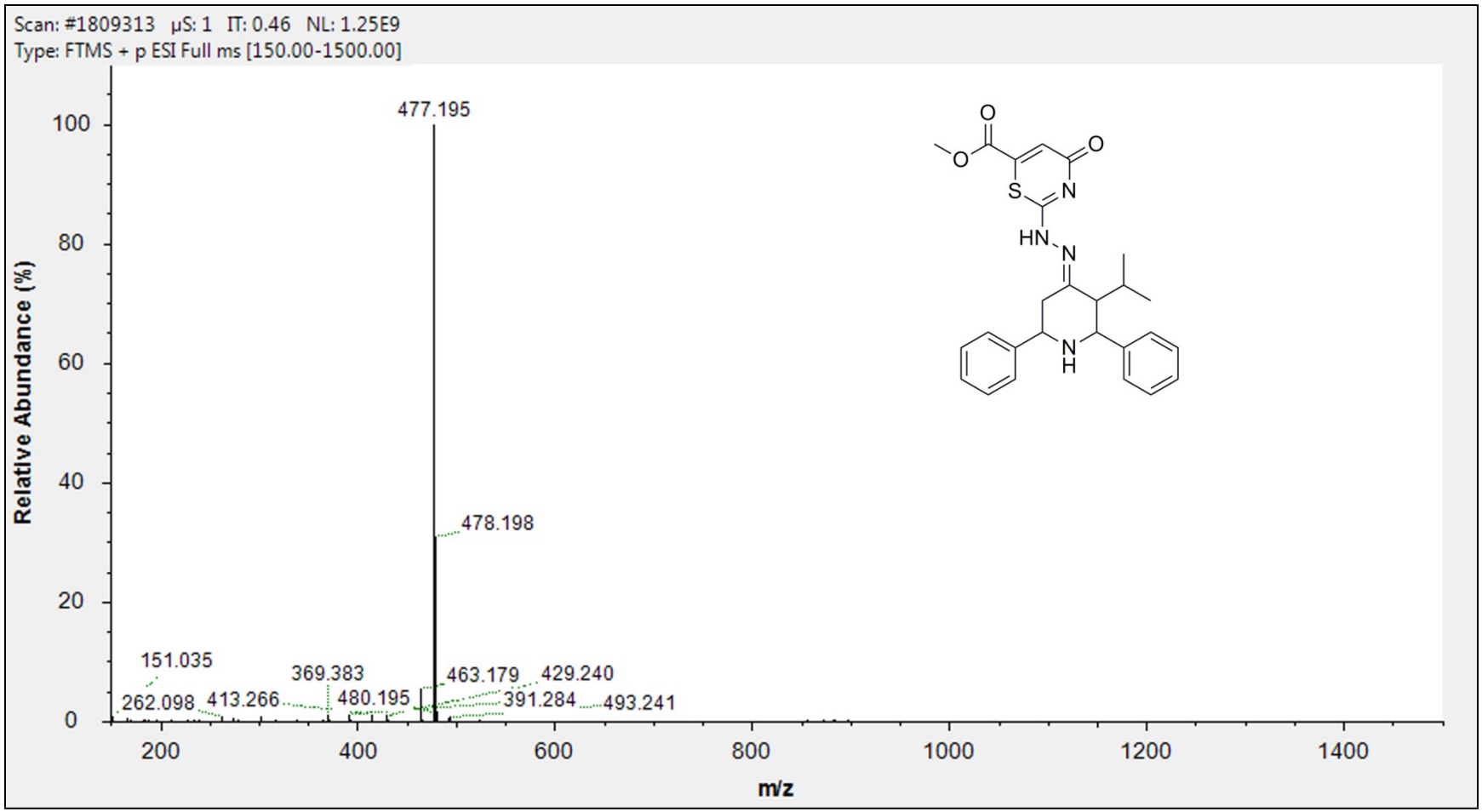


Fig. S 36 Mass spectrum of compound **24**

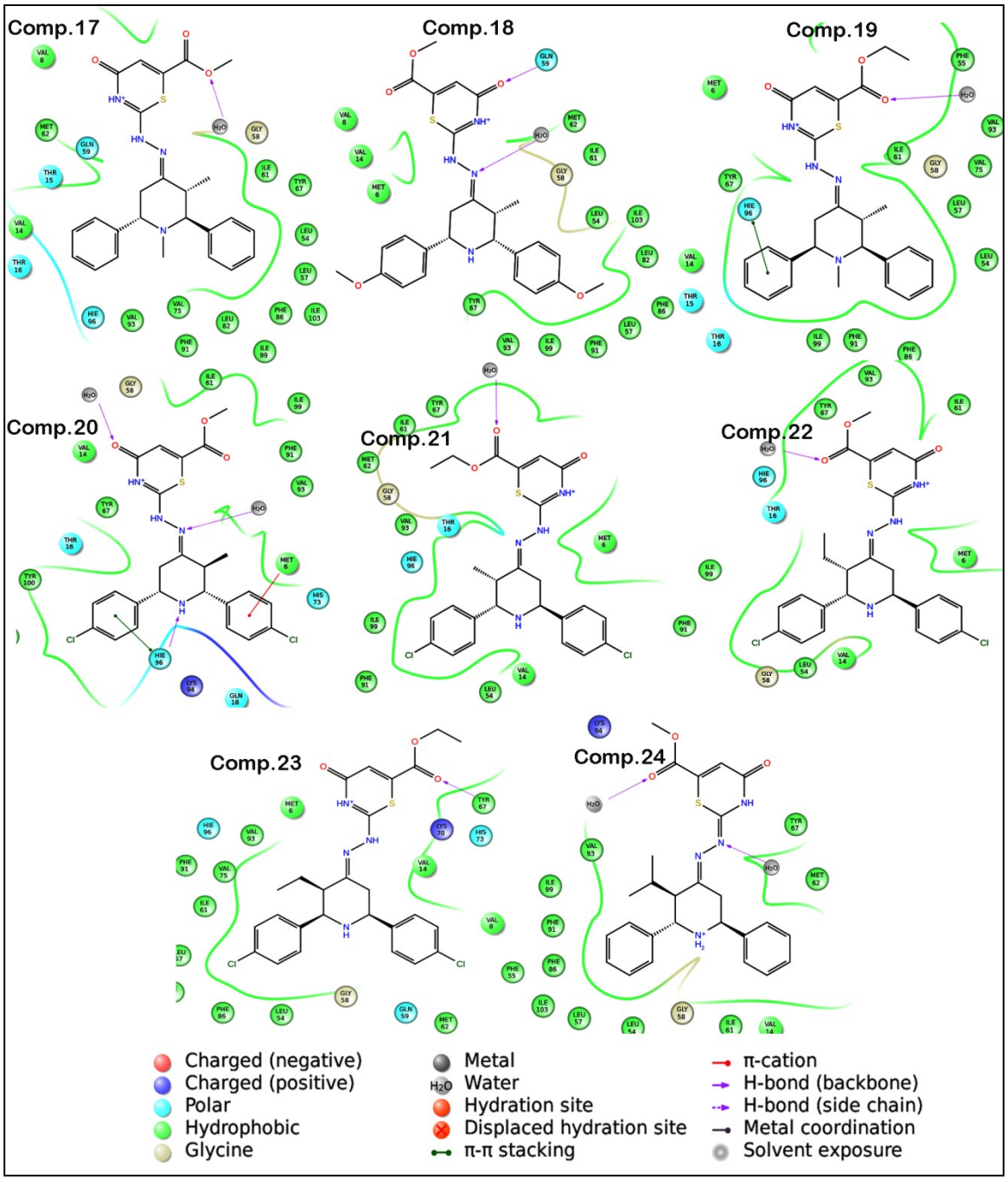


Fig. S 37 2D view of docking interactions of compounds **17**-**24** with MDM2 protein, PDB ID: 4ODE.

TABLE S1 Pictorial representation of HOMO-LUMO of the compounds **17** and **25**

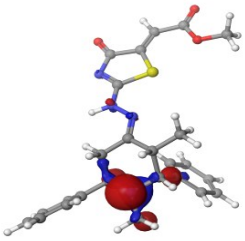
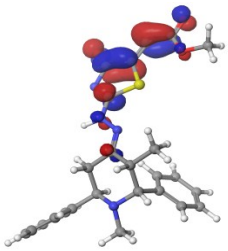
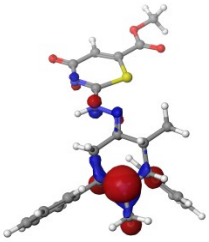
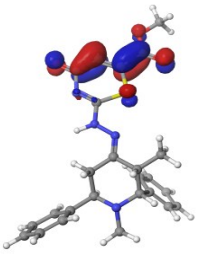
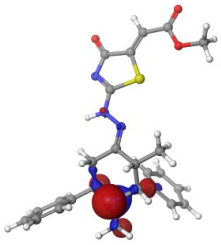
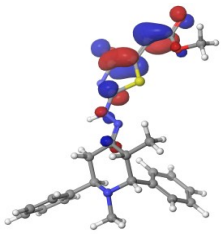
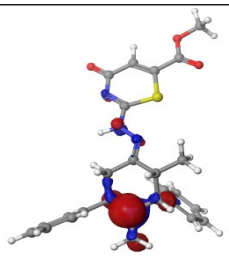
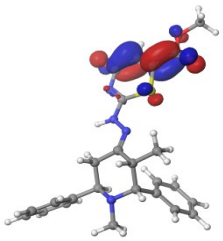
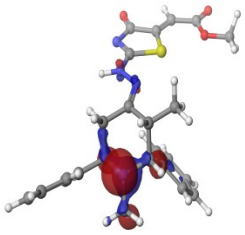
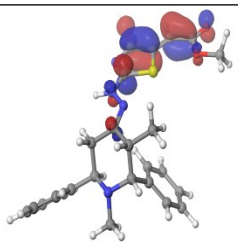
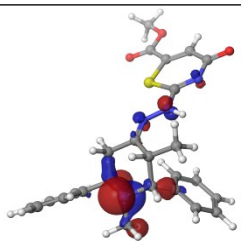
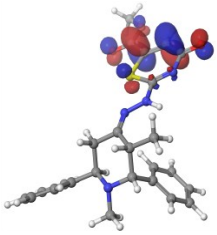
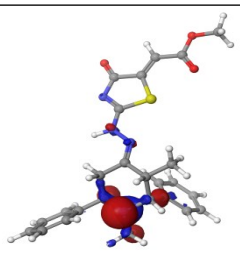
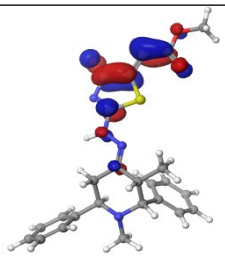
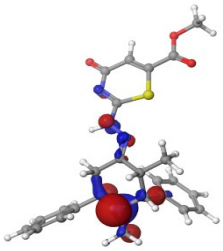
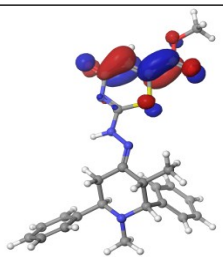
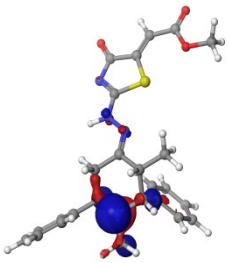
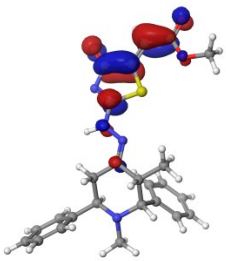
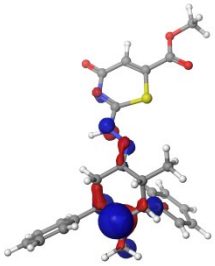
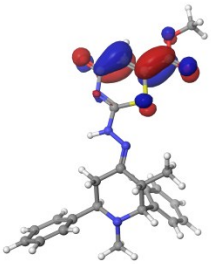
S.No	Theory and Basis set	Compound 25 (Five Membered Thiazolidinone Ring)		Compound 17 (Six Membered Thiazinone Ring)	
		HOMO	LUMO	HOMO	LUMO
1	**B3LYP 6-31G****	 -6.25323 eV	 -2.21995 eV	 -6.09471 eV	 -2.03881 eV
2	**B3LYP 6-311G****	 -6.45011 eV	 -2.40666 eV	 -6.29522 eV	 -2.22478 eV
3	**M06 6-31G****	 -6.68936 eV	 -2.04635 eV	 -6.49410 eV	 -1.82795 eV
4	**M06 6-311G****	 -6.83343 eV	 -2.17766 eV	 -6.74034 eV	 -2.01053 eV
5	**M06 6-311G 3DF 3PD**	 -9.63510 eV	 -2.21219 eV	 -9.47792 eV	 -1.99972 eV

Table S 2 Cartesian Coordinates of Compound **17** for B3LYP/6-31G** calculation

B3LYP/6-31G calculation of Compound 17**			
Cartesian Coordinates			
final geometry:			
		angstroms	
atom	x	y	z
N1	4.2403804901	-1.7958503752	1.2022057897
C2	3.7799636955	-3.1288274870	1.6667984190
C3	2.3507115468	-3.0082103733	2.2717849878
C4	1.4114907461	-2.3470252934	1.2894256606
C5	1.9309536511	-1.0519517556	0.7193427674
C6	3.3840820084	-1.1774428471	0.1802429188
C7	3.8631523101	0.2118655605	-0.2162747587
C8	5.6576273353	-1.8133356299	0.8332956213
C9	3.9650561429	-4.2677065031	0.6574613769
C10	1.8400445406	-4.3235647375	2.8616573694
N11	0.2830660423	-2.9107839585	1.0379488313
N12	-0.5951101905	-2.3279788817	0.1759030643
C13	4.1596105876	1.1752452033	0.7576198409
C14	4.5381425327	2.4634301399	0.3869764532
C15	4.6191851454	2.8103619302	-0.9636283763
C16	4.3247697235	1.8594480332	-1.9390155948
C17	3.9518637534	0.5670584621	-1.5650889639
C18	3.1258332858	-4.4778921161	-0.4491441004
C19	3.3791912425	-5.5054288824	-1.3583722238
C20	4.4743119151	-6.3500949790	-1.1827770060
C21	5.3127158959	-6.1627275580	-0.0848124154
C22	5.0558525264	-5.1341679586	0.8206808846
C23	-1.7569241488	-2.9569661085	-0.1748632901
N24	-2.5418447321	-2.3412755523	-0.9926049103
C25	-3.7526387086	-2.8604734973	-1.4492124191
C26	-4.1769264764	-4.2006947079	-0.9902355653
C27	-3.4937748052	-4.9890986731	-0.1411462703
S28	-1.9406438155	-4.5632951028	0.5953506627
O29	-4.4569864357	-2.2245658274	-2.2212185275
C30	-4.0569411055	-6.3298094131	0.2226233453
O31	-3.2454435701	-6.9905003655	1.0705063958
O32	-5.1073435966	-6.7667587002	-0.1944486912
C33	-3.6980075362	-8.2955792607	1.4749941094
H34	4.4358022706	-3.3689118173	2.5125576734
H35	2.4736428354	-2.2822233690	3.0901733158
H36	1.9318462179	-0.2994770099	1.5175172175
H37	1.3115700210	-0.6528881891	-0.0886871408
H38	3.3546833331	-1.7882635837	-0.7394687429
H39	6.0160329100	-0.7934036921	0.6887284585
H40	6.2311947835	-2.2607324036	1.6510697085
H41	5.8708473641	-2.3874102578	-0.0825168775

H42	0.8926937324	-4.1688555029	3.3834226072
H43	1.6745333623	-5.0758389568	2.0877656796
H44	2.5675451973	-4.7204909648	3.5772623819
H45	-0.4519884039	-1.4160738603	-0.2470079386
H46	4.1096107383	0.8982219792	1.8070494476
H47	4.7715756574	3.1986842156	1.1518228230
H48	4.9122407208	3.8156320493	-1.2520146667
H49	4.3884183790	2.1195308771	-2.9916731685
H50	3.7293984450	-0.1736306580	-2.3295820061
H51	2.2502651227	-3.8581731710	-0.5990052952
H52	2.7111576600	-5.6486512702	-2.2029630042
H53	4.6685878281	-7.1498368700	-1.8915222554
H54	6.1657477643	-6.8174828698	0.0695466571
H55	5.7161489228	-4.9997026241	1.6743617308
H56	-5.1206932266	-4.5647481179	-1.3828008229
H57	-2.9289481866	-8.6762402941	2.1457607660
H58	-4.6588790476	-8.2214976996	1.9890139995
H59	-3.8086729263	-8.9452566718	0.6039366191

Table S 3 Cartesian Coordinates of Compound **25** for B3LYP/6-31G** calculation

B3LYP/6-31G calculation of Compound 25**			
Cartesian Coordinates			
final geometry:			
		angstroms	
atom	x	y	z
N1	0.2074957798	2.9341996528	1.1750342485
C2	1.0454645928	4.0732126613	1.6265352771
C3	0.1407942403	5.1678440157	2.2649897852
C4	-0.9579442333	5.5661118621	1.3071731034
C5	-1.7389147407	4.4031581895	0.7508887521
C6	-0.8167953500	3.2858085761	0.1820907313
C7	-1.6901845847	2.0985968457	-0.1977441691
C8	2.0575618222	4.5875411095	0.5958933843
C9	1.0273508620	1.7881958177	0.7753193194
C10	0.9379812847	6.3354843596	2.8479632538
N11	-1.1283480456	6.8160641416	1.0592956391
N12	-2.1236443500	7.2104850101	0.2077054766
C13	-2.2215606255	8.5041675296	-0.1604113386
C14	-1.9585159257	1.8240805735	-1.5415322289
C15	-2.8108395524	0.7776614521	-1.8988280841
C16	-3.4006086734	-0.0096519896	-0.9116572222
C17	-3.1346527681	0.2541651086	0.4339887175
C18	-2.2886351592	1.3024344629	0.7881560049
C19	3.3999527122	4.2047341611	0.7311373864
C20	4.3673879993	4.5974132933	-0.1927396703
C21	4.0098730728	5.3905541013	-1.2820069587

C22	2.6822961925	5.7888857542	-1.4308095808
C23	1.7179352246	5.3942008742	-0.5030503470
N24	-3.1517949001	8.9188671402	-0.9636969456
C25	-3.0250447156	10.2841244234	-1.2081425887
C26	-1.8282293134	10.8951146970	-0.4726872077
S27	-1.0027209633	9.6588111808	0.4748808189
O28	-3.7563759594	10.9424708807	-1.9198205499
C29	-1.5280009434	12.1974533568	-0.6069143012
C30	-0.4128332289	12.9339089495	0.0113545976
O31	0.3585275132	12.1482491759	0.8045453554
O32	-0.1980795532	14.1165020765	-0.1672459022
C33	1.4693499921	12.8106244791	1.4299494414
H34	1.6404682579	3.6681941130	2.4540223258
H35	-0.3667788403	4.6426135482	3.0882819620
H36	-2.3337178075	3.9681651931	1.5631265810
H37	-2.4414163827	4.6858714121	-0.0382589194
H38	-0.3584352989	3.6652645302	-0.7483537459
H39	0.3956472076	0.9095805428	0.6395847966
H40	1.5958004226	1.9525344171	-0.1539363720
H41	1.7438795040	1.5700060185	1.5732440604
H42	0.2791805387	7.0203625247	3.3869291934
H43	1.6927438421	5.9606033130	3.5467849414
H44	1.4456491463	6.9066302049	2.0681762028
H45	-2.8151831317	6.5745562962	-0.1778562484
H46	-1.4946261226	2.4313702752	-2.3152393465
H47	-3.0088916526	0.5769792051	-2.9477732790
H48	-4.0618957473	-0.8259583549	-1.1872381252
H49	-3.5870631769	-0.3595321440	1.2077728153
H50	-2.0678189028	1.5003657013	1.8334408771
H51	3.6921275354	3.5880731144	1.5779790273
H52	5.3993532450	4.2854043298	-0.0593539682
H53	4.7590014827	5.7007745285	-2.0045986959
H54	2.3927921263	6.4174005937	-2.2682031013
H55	0.7020818067	5.7462444389	-0.6331620858
H56	-2.1742256317	12.7860350928	-1.2505805931
H57	1.9756893752	12.0450386015	2.0169054379
H58	2.1413858370	13.2255284804	0.6748753054
H59	1.1184646317	13.6212276418	2.0730889666

Table S 4 Cartesian Coordinates of Compound **17** for B3LYP/6-311G** calculation

B3LYP/6-311G calculation of Compound 17**			
Cartesian Coordinates			
final geometry:			
		angstroms	
atom	x	y	z
N1	-0.5720928596	4.3512604336	1.1294412766
C2	0.4008926541	5.3874723680	1.5523704233
C3	-0.3542891944	6.6072911033	2.1465206312
C4	-1.3940575261	7.1183427787	1.1787916994
C5	-2.3008750383	6.0527065274	0.6186140722
C6	-1.5459010318	4.7901514013	0.1221463066
C7	-2.5777818114	3.7137923119	-0.1907523444
C8	1.4787837846	5.7373624456	0.5215552123
C9	0.0940351629	3.0950384663	0.7796158896
C10	0.5820768120	7.6783564178	2.7046686320
N11	-1.4626679075	8.3802493160	0.9629805235
N12	-2.4195598885	8.8891335699	0.1423837679
C13	-2.4960998550	10.2336075258	-0.0892510801
N14	-3.4414950152	10.6481021481	-0.8575771624
C15	-3.6523851147	11.9825203771	-1.1889335508
C16	-2.7494557158	13.0086543841	-0.6229122608
C17	-1.7123782229	12.7648548506	0.1919552168
S18	-1.2219806631	11.1611989025	0.7550998417
O19	-4.5608003632	12.3124849772	-1.9293109863
C20	-0.8225679648	13.8332651877	0.7416594281
O21	-1.1769364471	15.0590118724	0.3301076524
O22	0.1091179034	13.6046600635	1.4749832281
C23	-0.3628257868	16.1411208578	0.8224125318
C24	-2.8964699124	3.4070904657	-1.5140685016
C25	-3.8831812095	2.4679104294	-1.8117614433
C26	-4.5599041613	1.8188296922	-0.7840723497
C27	-4.2444556646	2.1136232390	0.5422864529
C28	-3.2637904211	3.0552087892	0.8358654008
C29	2.7724754448	5.2355194874	0.7083139934
C30	3.7922596364	5.4902842151	-0.2047036212
C31	3.5369278644	6.2600114873	-1.3357125199
C32	2.2591216060	6.7746044182	-1.5362813609
C33	1.2429668810	6.5184825030	-0.6184579735
H34	0.9324441175	4.9370788164	2.3967796757
H35	-0.9267004693	6.1785455062	2.9816718917
H36	-2.9861333578	5.7444035602	1.4163316581
H37	-2.9200729358	6.4084022223	-0.2077381201
H38	-1.0456654514	5.0427500315	-0.8273646935
H39	-0.6423667375	2.2993692393	0.6753203415
H40	0.6768740966	3.1515526897	-0.1524059079
H41	0.7751473668	2.8193822740	1.5882199255

H42	0.0152658807	8.4489802919	3.2286384672
H43	1.2854589539	7.2280616266	3.4104413420
H44	1.1541486041	8.1674822092	1.9157488109
H45	-3.1443018441	8.3327485379	-0.2985560769
H46	-2.9687963512	14.0288763741	-0.9103650940
H47	-0.7916087100	17.0419906866	0.3907373531
H48	-0.4001920195	16.1777324497	1.9117770253
H49	0.6718121753	16.0124961293	0.5023643124
H50	-2.3658993445	3.9032007807	-2.3204100658
H51	-4.1179473713	2.2426605767	-2.8458900035
H52	-5.3256657553	1.0862827224	-1.0123181311
H53	-4.7640174274	1.6077552815	1.3485022552
H54	-3.0077932935	3.2733168563	1.8668126246
H55	2.9858882035	4.6375201491	1.5888142699
H56	4.7846295979	5.0898958992	-0.0299797103
H57	4.3266774036	6.4634176482	-2.0496691781
H58	2.0510000472	7.3866221981	-2.4066555436
H59	0.2704113400	6.9595547602	-0.7897844958

Table S 5 Cartesian Coordinates of Compound **25** for B3LYP/6-311G** calculation

B3LYP/6-311G calculation of Compound 25**			
Cartesian Coordinates			
final geometry:			
		angstroms	
atom	x	y	z
N1	-0.8266795510	-0.7938224394	1.1549265661
C2	0.0538753306	0.3343355218	1.5417168180
C3	-0.8067720587	1.5122210690	2.0743487073
C4	-1.8703875222	1.8969800677	1.0742120769
C5	-2.6789665472	0.7380695672	0.5495575466
C6	-1.8166792573	-0.4799372363	0.1178463115
C7	-2.7511407560	-1.6517674291	-0.1573357286
C8	1.1150744392	0.7262013881	0.5086425420
C9	-3.0172803426	-2.0484295718	-1.4684925817
C10	-3.9132620750	-3.0839488869	-1.7330227897
C11	-4.5498034622	-3.7394330253	-0.6839179222
C12	-4.2862054679	-3.3543168948	0.6305371032
C13	-3.3967397856	-2.3173400187	0.8909228384
C14	2.4399581608	0.3289841500	0.7266274924
C15	3.4491080491	0.6240088018	-0.1860437378
C16	3.1516750921	1.3302727430	-1.3477590811
C17	1.8419789198	1.7412302808	-1.5800827588
C18	0.8361925443	1.4444330402	-0.6626976682
N19	-2.0309268708	3.1405234003	0.8079763296
C20	0.0313716324	2.6772386555	2.5993414292
C21	-0.0584990885	-2.0082731982	0.8720887570

N22	-3.0168500651	3.5378574473	-0.0503800675
C23	-3.1743591106	4.8470572479	-0.3341449328
N24	-4.1052114132	5.2671226132	-1.1268088644
C25	-4.0655066930	6.6510511334	-1.2629938217
C26	-2.9353339409	7.2756398855	-0.4378460102
S27	-2.0481319432	6.0213140858	0.4221566213
O28	-4.8144787973	7.3120114131	-1.9402625111
C29	-2.7291600880	8.5996913841	-0.4350926909
C30	-1.6944814927	9.3462626833	0.2983069503
O31	-0.8989952061	8.5377552203	1.0406726861
O32	-1.5614950287	10.5462224129	0.2499546940
C33	0.1380675659	9.1944946721	1.7890409533
H34	0.6076869797	-0.0342653830	2.4109867076
H35	-1.3564155288	1.0724714968	2.9188178438
H36	-3.3476152591	0.4096235123	1.3530457714
H37	-3.3135749251	1.0048450313	-0.2985074995
H38	-1.3248690691	-0.2284429514	-0.8363571835
H39	-2.5158346911	-1.5483117164	-2.2909812879
H40	-4.1077536209	-3.3793217460	-2.7578583747
H41	-5.2438886180	-4.5470653343	-0.8863220128
H42	-4.7740035887	-3.8649323413	1.4532915981
H43	-3.1786786514	-2.0297602695	1.9135163429
H44	2.6862432606	-0.2185771505	1.6309457549
H45	4.4659041888	0.3044777560	0.0127353973
H46	3.9329057169	1.5647019518	-2.0615492577
H47	1.6000504892	2.3033625116	-2.4750352237
H48	-0.1641718005	1.8047752552	-0.8611128023
H49	-0.6039984529	3.4200483373	3.0833944006
H50	0.7561854531	2.3131273535	3.3325423387
H51	0.5760200224	3.1773455957	1.7978934801
H52	-0.7287012377	-2.8632827265	0.7949391184
H53	0.5337865387	-1.9476618757	-0.0535982977
H54	0.6279161309	-2.1927506746	1.7017690656
H55	-3.6842056611	2.8997178466	-0.4714418389
H56	-3.3945135733	9.2046300434	-1.0402132143
H57	0.6643726731	8.4013509488	2.3152021766
H58	0.8135122755	9.7260992693	1.1171959369
H59	-0.2943451997	9.9050698190	2.4949753027

Table S 6 Cartesian Coordinates of Compound **17** for M06/6-31G** calculation

M06/6-31G calculation of Compound 17**			
Cartesian Coordinates			
final geometry:			
		angstroms	
atom	x	y	z
N1	-1.0535743915	-0.6646715602	0.9311166729
C2	0.2045358425	0.0563695003	1.1578802812
C3	-0.0213754798	1.2790071067	2.0757524315
C4	-1.1001098012	2.1470403595	1.4732490533
C5	-2.3705774041	1.3831044613	1.2691241299
C6	-2.1525064980	0.1362564291	0.3966912129
C7	-3.4440720719	-0.6444802685	0.3522648167
C8	1.0114000055	0.3824427141	-0.0893520838
C9	-0.8326170031	-1.8788463540	0.1633233791
C10	1.3072283664	1.8904311204	2.4991197588
N11	-1.1123487471	3.3645895097	1.0716689167
N12	-0.0202430304	4.1635386352	1.1242371355
C13	-0.0884560842	5.4364442332	0.6379813001
N14	0.9806971790	6.1487504822	0.6878838869
C15	1.0672228731	7.4558329064	0.2291874656
C16	-0.1352125593	8.0800206081	-0.3544457168
C17	-1.3293802467	7.4857545996	-0.4853245702
S18	-1.7085839147	5.8390566875	0.0143530951
C19	-2.5188103114	8.1475977147	-1.0867812265
O20	-2.2686742658	9.4011305224	-1.4739321558
O21	-3.5895056627	7.5983031418	-1.2076413895
C22	-3.3789270404	10.0788839570	-2.0606089271
C23	-4.2709592860	-0.5662270366	-0.7641145116
C24	-5.4979930999	-1.2213253527	-0.7833947925
C25	-5.9047735376	-1.9667446505	0.3155626986
C26	-5.0811930684	-2.0531457342	1.4345579235
C27	-3.8606875836	-1.3928177854	1.4543458840
C28	2.2073049611	-0.3049610710	-0.3037993635
C29	2.9864717542	-0.0709141309	-1.4300629185
C30	2.5783540358	0.8644451971	-2.3724606326
C31	1.3925061798	1.5613988872	-2.1741489439
C32	0.6165771485	1.3263715495	-1.0449855289
O33	2.1068151168	8.0847111639	0.2993491348
H34	0.8276097381	-0.6373972605	1.7473594410
H35	-0.4949023150	0.8556881480	2.9776607368
H36	-2.7599004425	1.0453540477	2.2413771286
H37	-3.1255560033	2.0274553198	0.8069401792
H38	-1.9331041712	0.4704999697	-0.6399626934
H39	-1.7191296810	-2.5178654639	0.2078736664
H40	-0.6008662982	-1.6851546021	-0.8999188035
H41	0.0087796924	-2.4343355596	0.5942990995

H42	1.1745809784	2.7223535332	3.1992995913
H43	1.9033436093	1.1301867632	3.0175737776
H44	1.9131490631	2.2180812373	1.6451925377
H45	0.8935067854	3.8704677553	1.4557759820
H46	-0.0101896431	9.1033866816	-0.6984600677
H47	-3.0194570327	11.0745585083	-2.3203946526
H48	-3.7238649622	9.5498673398	-2.9537415247
H49	-4.2087077922	10.1430991615	-1.3508109220
H50	-3.9479769484	0.0156915898	-1.6271456731
H51	-6.1352924177	-1.1514965535	-1.6618312502
H52	-6.8619212165	-2.4827463721	0.3015794898
H53	-5.3937798203	-2.6391490534	2.2959777574
H54	-3.2024762809	-1.4639089569	2.3195952230
H55	2.5317873073	-1.0411387127	0.4325100939
H56	3.9148543211	-0.6197422816	-1.5699497784
H57	3.1835637221	1.0540383999	-3.2555918949
H58	1.0672490807	2.3015453409	-2.9015287254
H59	-0.2957157634	1.9018753630	-0.9106271285

Table S 7 Cartesian Coordinates of Compound **25** for M06/6-31G** calculation

M06/6-31G calculation of Compound 25**			
Cartesian Coordinates			
final geometry:			
angstroms			
atom	x	y	z
N1	-0.7709369981	-0.7424002530	1.1338732969
C2	-0.0375055481	0.4201048398	1.6620818492
C3	-1.0022346435	1.3468377647	2.4343154412
C4	-2.1414658892	1.7206059759	1.5341770142
C5	-2.8549382721	0.5488591454	0.9395810585
C6	-1.8728549744	-0.4113054548	0.2376992701
C7	-2.6421055818	-1.6355289138	-0.1972390130
C8	0.1355866957	-1.7163660957	0.5466470389
C9	0.8537794135	1.1349924684	0.6567860169
C10	-0.2844138583	2.5229403116	3.0681025273
N11	-2.3364474222	2.9641208236	1.3020468950
N12	-3.3006400832	3.3531711644	0.4207789480
C13	-3.2637868109	4.6121402065	-0.0544585234
N14	-4.1335039099	5.0688711346	-0.8919890371
C15	-3.8302902617	6.3790259629	-1.2425002670
C16	-2.5686001075	6.8816974730	-0.5498572640
S17	-1.8998829952	5.6361405128	0.4901183273

O18	-4.4639324740	7.0685257338	-2.0057383436
C19	-2.1147978285	8.1192875036	-0.7822744868
C20	-0.9209188136	8.7531437968	-0.2115555759
O21	-0.2584109587	7.9374391895	0.6342585135
C22	0.9101929012	8.5031389479	1.2187945755
O23	-0.5619097359	9.8793638099	-0.4663163588
C24	-2.9817143470	-1.8087695720	-1.5353712069
C25	-3.7475107569	-2.8994922595	-1.9353025169
C26	-4.1749408186	-3.8289829427	-0.9963419288
C27	-3.8347577488	-3.6647216520	0.3437274070
C28	-3.0762115801	-2.5729067418	0.7414680447
C29	2.2348921496	0.9511142728	0.7548995002
C30	3.1141764988	1.5396266051	-0.1456304971
C31	2.6253537653	2.3357848201	-1.1737848894
C32	1.2550468762	2.5386680862	-1.2845577763
C33	0.3788752582	1.9461679185	-0.3822915251
H34	0.6411401919	0.0042520893	2.4242935665
H35	-1.4256848304	0.7026185552	3.2234165800
H36	-3.3507675239	-0.0082339266	1.7477728773
H37	-3.6341677843	0.8199307270	0.2171521845
H38	-1.5004184019	0.0868826994	-0.6827291327
H39	-0.3874026890	-2.6603291921	0.3696682496
H40	0.5738291353	-1.3797608351	-0.4102225875
H41	0.9587844265	-1.9102833650	1.2438408397
H42	-0.9637271751	3.1038544721	3.6990150588
H43	0.5464631598	2.1654364980	3.6874599841
H44	0.1210295018	3.2003031240	2.3094273984
H45	-4.0312428815	2.7405824885	0.0664971728
H46	-2.6880258042	8.7314736614	-1.4758694351
H47	1.3302928218	7.7319156445	1.8648310689
H48	1.6289023981	8.7881577438	0.4446240554
H49	0.6568764229	9.3945372136	1.8005189112
H50	-2.6383285425	-1.0824133015	-2.2718338661
H51	-4.0055077609	-3.0243606579	-2.9842806994
H52	-4.7705008369	-4.6840898240	-1.3069411110
H53	-4.1625667567	-4.3938703310	1.0810729687
H54	-2.7902781004	-2.4449118432	1.7850293247
H55	2.6277657715	0.3287433967	1.5595148090
H56	4.1842690746	1.3757922602	-0.0414287295
H57	3.3075797726	2.8010430602	-1.8808299889
H58	0.8585561666	3.1701231056	-2.0762595544

H59	-0.6834535351	2.1500838741	-0.4884968220

Table S 8 Cartesian Coordinates of Compound **17** for M06/6-311G** calculation

M06/6-311G calculation of Compound 17**			
Cartesian Coordinates			
final geometry:			
angstroms			
atom	x	y	z
N1	-3.2710093143	-2.1738792113	1.1299415661
C2	-2.3511499707	-1.1225554706	1.5902089968
C3	-3.1400658049	0.0298272611	2.2373474549
C4	-4.1910188430	0.5301523145	1.2941823263
C5	-5.0707471358	-0.5426919750	0.7356548183
C6	-4.2784458505	-1.7350276351	0.1743471310
C7	-5.2591021536	-2.8343403746	-0.1610329786
C8	-1.3216694451	-0.6768589440	0.5663908417
N9	-4.2519067618	1.7837768458	1.0624773334
N10	-5.1771242197	2.2829765001	0.2157629600
C11	-5.2010574008	3.6167342096	-0.0678019378
C12	-5.6048070462	-3.0843183667	-1.4825626670
C13	-6.5530455904	-4.0494414790	-1.7966402053
C14	-7.1596327055	-4.7786718087	-0.7869812768
C15	-6.8145607911	-4.5394665573	0.5376589316
C16	-5.8736927522	-3.5721220686	0.8483702461
C17	-0.0023206928	-1.0955748228	0.7255247948
C18	0.9829775560	-0.7531032679	-0.1880039000
C19	0.6636310972	0.0237553093	-1.2904030408
C20	-0.6421933644	0.4574065727	-1.4626377124
C21	-1.6239238426	0.1135926216	-0.5449305751
C22	-2.2352223209	1.1084075527	2.7976579827
C23	-2.5496128357	-3.3455322539	0.6641263640
N24	-6.1086111564	4.0354271839	-0.8671017403
C25	-6.2594664708	5.3566294647	-1.2595840512
C26	-5.3143397525	6.3537821519	-0.7269740350
C27	-4.3103740695	6.0969698616	0.1162313612
S28	-3.9071131994	4.5108769474	0.7667291422
O29	-7.1380052648	5.6945936819	-2.0191462590
C30	-3.3809385451	7.1409837905	0.6281539379
O31	-3.6617506842	8.3501013708	0.1463085599

O32	-2.4819578972	6.9056304573	1.3901131469
C33	-2.8080401918	9.3983751217	0.5980140291
H34	-1.7812068114	-1.5847596694	2.4100661537
H35	-3.6869673319	-0.4497732857	3.0667046409
H36	-5.7072696531	-0.9152044421	1.5510993802
H37	-5.7459010383	-0.1931552090	-0.0529587715
H38	-3.8061004109	-1.4216990698	-0.7794038263
H39	-5.9079666223	1.7309515516	-0.2275717013
H40	-5.1219519578	-2.5181617365	-2.2760499507
H41	-6.8134375793	-4.2336903383	-2.8341791424
H42	-7.8985165300	-5.5358125027	-1.0293758669
H43	-7.2828149862	-5.1125907988	1.3319410411
H44	-5.5869399224	-3.3916697472	1.8816467321
H45	0.2561878234	-1.7048525333	1.5894680767
H46	2.0027116777	-1.0930176247	-0.0360759285
H47	1.4296407351	0.2964413266	-2.0091409273
H48	-0.9008769766	1.0770713562	-2.3155089627
H49	-2.6283197616	0.4955920818	-0.6954456010
H50	-2.8088935635	1.8410372344	3.3706705183
H51	-1.4827009079	0.6633443359	3.4574162452
H52	-1.7143703756	1.6502795394	2.0032604310
H53	-3.2294901900	-4.1944651212	0.5617796588
H54	-2.0494499723	-3.1870974697	-0.3080633654
H55	-1.7833283811	-3.6134303149	1.3980295520
H56	-5.4733381292	7.3720225011	-1.0661010955
H57	-3.1684351318	10.3054931118	0.1169364164
H58	-2.8608293528	9.4948114977	1.6851086383
H59	-1.7721728772	9.1994710230	0.3128834912

Table S 9 Cartesian Coordinates of Compound **25** for M06/6-311G** calculation

M06/6-311G calculation of Compound 25**			
Cartesian Coordinates			
final geometry:			
angstroms			
atom	x	y	z
N1	0.4052942635	-6.1283641517	1.1074654596
C2	1.2503658006	-5.0027062279	1.5325688186
C3	0.3862882060	-3.8985570266	2.1672242127
C4	-0.7099913446	-3.4952227195	1.2287989090

C5	-1.5134132385	-4.6415132469	0.7019068472
C6	-0.6428601766	-5.7861710668	0.1567296197
C7	-1.5442712377	-6.9621923792	-0.1388338554
C8	2.2307942585	-4.5042716621	0.4856377063
C9	1.2052754564	-7.2545090158	0.6578377672
C10	1.2158801650	-2.7469406469	2.6975475674
N11	-0.8664519206	-2.2529620627	0.9824577372
N12	-1.8474517391	-1.8449596726	0.1389522838
C13	-1.9682459749	-0.5386159768	-0.1574284712
N14	-2.8860186321	-0.1035428587	-0.9488080112
C15	-2.7984755532	1.2715870235	-1.0944393828
C16	-1.6523890363	1.8507509399	-0.2775353900
S17	-0.7963768072	0.5926680670	0.5864314132
O18	-3.5156433611	1.9575238722	-1.7700097270
C19	-1.3933509432	3.1592933905	-0.2680100154
C20	-0.2954333134	3.7236699858	0.5166820071
O21	0.4619371382	3.0840343510	1.2052711838
O22	-0.2312916048	5.0539817681	0.3777311051
C23	0.8086087105	5.6918331409	1.1087543751
C24	-1.8791531098	-7.2764240487	-1.4492601257
C25	-2.7538683973	-8.3192215314	-1.7263170921
C26	-3.2961787969	-9.0619689493	-0.6903239400
C27	-2.9606266669	-8.7586325884	0.6236286228
C28	-2.0934313851	-7.7144431438	0.8972538390
C29	3.5794599334	-4.8200654516	0.6346003906
C30	4.5244582991	-4.4246853805	-0.2997298848
C31	4.1339160551	-3.6973005436	-1.4129032258
C32	2.7972671519	-3.3657443891	-1.5753001858
C33	1.8561139491	-3.7624012557	-0.6367349614
H34	1.8627660210	-5.4033178792	2.3539939608
H35	-0.1165822877	-4.4007171355	3.0108450252
H36	-2.1121775543	-5.0396982878	1.5334680829
H37	-2.2212002425	-4.3614255770	-0.0860419686
H38	-0.2072165989	-5.4615007172	-0.8106107675
H39	0.5888551248	-8.1533972748	0.5846747177
H40	1.6800187443	-7.0823999634	-0.3246306886
H41	1.9984305481	-7.4475948189	1.3865578854
H42	0.5971479702	-2.0468465377	3.2639217308
H43	2.0046770981	-3.1251856637	3.3565022736
H44	1.6887555269	-2.1844178606	1.8879609807
H45	-2.5271613319	-2.4727756696	-0.2847232178

H46	-2.0234871762	3.8137895433	-0.8624414832
H47	0.7227572026	6.7547339944	0.8897141132
H48	0.6933874819	5.5132218318	2.1810585655
H49	1.7869580511	5.3163635076	0.7974999592
H50	-1.4454862733	-6.6998820904	-2.2633568789
H51	-3.0065608515	-8.5537216546	-2.7555578391
H52	-3.9770986671	-9.8797884106	-0.9036949951
H53	-3.3776777698	-9.3423549765	1.4384482641
H54	-1.8126080059	-7.4839923431	1.9221655836
H55	3.8939365508	-5.3896211659	1.5069422086
H56	5.5686560696	-4.6839197983	-0.1554935435
H57	4.8681617123	-3.3829609917	-2.1475978790
H58	2.4822644024	-2.7844042123	-2.4361861493
H59	0.8243091920	-3.4590549047	-0.7808432603

Table S 10 Cartesian Coordinates of Compound **17** for M06/6-311G-3DF-3PD calculation

M06/6-311G-3DF-3PD calculation of Compound 17			
Cartesian Coordinates			
final geometry:			
		angstroms	
atom	x	y	z
N1	4.2031946874	-1.7925657029	1.1595720872
C2	3.7327805928	-3.1025299977	1.6231889164
C3	2.3167540641	-2.9828048685	2.2094691254
C4	1.4005332971	-2.3353692961	1.2212962830
C5	1.9127292220	-1.0442318400	0.6749449113
C6	3.3596105526	-1.1424077844	0.1707945619
C7	3.8418988440	0.2480404438	-0.1598404492
C8	5.5933926906	-1.8376488698	0.7513997097
C9	3.8998459299	-4.2339958350	0.6272928887
C10	1.8118485219	-4.2941514140	2.7688960238
N11	0.3006122438	-2.9115745942	0.9408389952
N12	-0.5567671688	-2.3700592177	0.0536276890
C13	4.1237105967	1.1630437401	0.8479414721
C14	4.5175222700	2.4502062220	0.5360806370
C15	4.6290644206	2.8436950791	-0.7888063949
C16	4.3501918168	1.9403118357	-1.7970064454
C17	3.9618101897	0.6478998779	-1.4809500502
C18	3.1233045529	-4.3756198598	-0.5213547006
C19	3.3479763604	-5.4149618985	-1.4075883747
C20	4.3495253677	-6.3386445383	-1.1656637293
C21	5.1230100601	-6.2184195084	-0.0256459940
C22	4.8955747643	-5.1766575887	0.8561358806

C23	-1.7082644061	-3.0175375167	-0.2742579988
N24	-2.4851629388	-2.4550692208	-1.1175506232
C25	-3.6867511127	-2.9872532720	-1.5551546961
C26	-4.1059060715	-4.2880728543	-1.0164182798
C27	-3.4236039072	-5.0151920500	-0.1317955255
S28	-1.8850579859	-4.5620699174	0.5678814063
O29	-4.3762298896	-2.4053668743	-2.3569965243
C30	-3.9898466563	-6.3203761789	0.3151873180
O31	-3.1904967179	-6.9210305380	1.1990550171
O32	-5.0278238289	-6.7730380249	-0.0685248449
C33	-3.6488607455	-8.1758155073	1.6834691170
H34	4.3819979995	-3.3518287391	2.4710757580
H35	2.4271831819	-2.2608179836	3.0309957750
H36	1.8884047254	-0.3036539226	1.4819468078
H37	1.3063252035	-0.6396739038	-0.1374335367
H38	3.3569550976	-1.7130630409	-0.7764856726
H39	5.9930079659	-0.8297085444	0.6523329423
H40	6.1763907342	-2.3589652419	1.5111862482
H41	5.7432356258	-2.3586651869	-0.2066346140
H42	0.8744299276	-4.1535362913	3.3053421342
H43	1.6300062706	-5.0236135271	1.9796235431
H44	2.5459652065	-4.7146876288	3.4584105024
H45	-0.4141988779	-1.4751259092	-0.4035066537
H46	4.0510475099	0.8474506194	1.8829909445
H47	4.7405604500	3.1525573747	1.3293500663
H48	4.9363048333	3.8527478972	-1.0319293339
H49	4.4390695274	2.2379073789	-2.8340485235
H50	3.7516766633	-0.0636570175	-2.2723966185
H51	2.3139518048	-3.6876719209	-0.7285404602
H52	2.7288947199	-5.5055645463	-2.2911546752
H53	4.5214992908	-7.1508995291	-1.8600841879
H54	5.9058321580	-6.9375290644	0.1799215478
H55	5.5066611103	-5.0888230900	1.7486908077
H56	-5.0509836132	-4.6740874412	-1.3791993740
H57	-2.8965488964	-8.5264086936	2.3819779398
H58	-4.6098433488	-8.0639068369	2.1833321616
H59	-3.7650986226	-8.8822608245	0.8629433932

Table S 11 Cartesian Coordinates of Compound **25** for M06/6-311G-3DF-3PD calculation

M06/6-311G-3DF-3PD calculation of Compound 25			
Cartesian Coordinates			
final geometry:			
		angstroms	
atom	x	y	z
N1	0.0798585784	0.0366694130	1.0998632208
C2	1.2483859497	0.8983458956	1.3107685760

C3	0.4594041945	-1.2604901748	0.5751077252
C4	-1.0118029212	0.6372123051	0.3525552056
C5	0.8335979468	2.1939628406	2.0261316610
C6	2.1239358176	1.1130737903	0.0911027892
C7	-0.2816090264	2.8632974354	1.2884450586
C8	2.0144803196	3.0889301190	2.3299141480
C9	-1.4381963791	1.9648659098	0.9972909602
N10	-0.1570560921	4.0952941351	0.9902133607
C11	-2.2144760472	-0.2704910721	0.2858980182
C12	-2.8351274835	-0.5191487249	-0.9277165198
C13	-2.7413952500	-0.8400050489	1.4397184669
C14	3.3548921337	0.4686894827	0.0390880351
C15	1.7650123010	1.9147727411	-0.9912091558
N16	-1.1438458692	4.7440771806	0.3256141001
C17	-0.9779225282	6.0290607816	-0.0261110144
N18	-1.8874397700	6.6844273719	-0.6538876857
S19	0.5558749594	6.8143355869	0.3991743450
C20	-1.4778917052	7.9822481937	-0.9041917824
C21	-0.0768541249	8.2454059067	-0.3641164581
O22	-2.1158524138	8.8213699624	-1.4712589594
C23	0.4898952074	9.4407184762	-0.5106294627
C24	1.8157136626	9.8669558399	-0.0599154425
O25	2.4871179319	8.8865489526	0.5690977844
O26	2.2615233467	10.9676292149	-0.2295469224
C27	3.7817690374	9.2386445963	1.0310600393
C28	-3.9689423637	-1.3135421276	-0.9933752709
C29	-4.4876101928	-1.8737245661	0.1588660711
C30	-3.8683394702	-1.6369877675	1.3767384769
C31	4.1963664230	0.6011403043	-1.0513304915
C32	3.8192182535	1.3912840679	-2.1217107856
C33	2.6021712766	2.0489727999	-2.0852380642
H34	1.8714911715	0.3546767895	2.0307475355
H35	-0.3691793067	-1.9617082156	0.6589432850
H36	0.7688601754	-1.2231157747	-0.4804856711
H37	1.2945898492	-1.6535308075	1.1555892711
H38	-0.7072803470	0.8418904884	-0.6905699665
H39	0.3922045800	1.8476329512	2.9718726533
H40	1.7183483940	3.9210792811	2.9668544222
H41	2.7915837049	2.5195665143	2.8425807685
H42	2.4451149426	3.5094316537	1.4213587100
H43	-2.1974299741	2.4149472005	0.3552321928
H44	-1.9305782460	1.7320870395	1.9476540787
H45	-2.4228995185	-0.0867715599	-1.8332347587
H46	-2.2461181574	-0.6666332330	2.3889387096
H47	3.6579389331	-0.1528091820	0.8756800092
H48	0.8337320614	2.4655789613	-0.9850914359
H49	-2.0272111257	4.3140340623	0.0714407942
H50	-0.0885815386	10.2002994122	-1.0241859179
H51	4.1886731442	8.3536782005	1.5096639085

H52	4.4158678933	9.5457930986	0.2002940218
H53	3.7252383583	10.0620872848	1.7419058426
H54	-4.4436577790	-1.4970984395	-1.9487147233
H55	-5.3709721129	-2.4973246058	0.1107114268
H56	-4.2667960596	-2.0788042347	2.2813222833
H57	5.1488413196	0.0866312903	-1.0628894493
H58	4.4720792045	1.4998798912	-2.9780398969
H59	2.3020601529	2.6798521708	-2.9122757343