Amidosquaramides – A new anion binding motif with pH sensitive anion transport properties

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Supporting Information

^{1}H NMR Anion Binding Studies: Both the tetrabutylammonium salts and the receptors were lyophilised before use. Solutions of the TBA salts were made up in DMSO-d_6, which was dried over 3Å molecular sieves before use, to a concentration of 300 mM. An aliquot of stock solution of receptor in DMSO-d_6 was diluted to 1 mL (2.5 mM). 600 µL of this solution was added to an NMR tube and the ^{1}H NMR spectrum was recorded. Subsequent additions of aliquots of TBA salt solutions were added to the NMR tube and shaken vigorously to ensure homogenisation. This process was repeated up to 22 equivalents of halide was reached.

The ^{1}H NMR spectra were analysed and processed, and stackplots were generated using MestReNova 6.0.2 software. A global fitting analysis assuming a 1:1 binding model was employed to provide the binding constant (K_a/M^{-1}), by fitting of the chemical shift changes of the NH signals as function of anion concentration using the open access BindFit software program.[1,2]

UV/Vis pH-spectrophotometric titrations: pK_a values were experimentally determined using the wavelength of maximum difference in absorbance between the UV/Vis spectra of the

neutral and anionic species. The absorbance of each receptor was measured in a solution of DMSO/H_2O (9:1) containing 0.1 M $TBAPF_6$ between approximately pH 2.5 to 12.5. The solutions were initially acidified using HNO_3 and gradually basified by aliquots of either 1 M or 0.1 M NaOH. The absorbance values of maximal difference were plotted against pH values. A four parameter sigmoid curve using Sigma Plot was fitted through the data points with the point of inflexion corresponding to the pK_a value.

Anion transport assays:

The methods for the anion transport assays were adapted from methods previously reported by Gale *et al*.[3]

Preparation of POPC vesicles

The internal solution (NaCl 487 mM, sodium phosphate 5 mM) and external solution ($NaNO_3$ 487 mM, sodium phosphate 5 mM) were prepared using Milli-Q water to prevent ion contamination and buffered to pH 7.20. 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) (118 mg) and cholesterol (26 mg) were dissolved in $CHCl_3$ (5 mL) in a 25 mL round-bottomed flask. The $CHCl_3$ was slowly gently removed using a rotary evaporator to form a thin lipid film, which was then dried under vacuum overnight. The lipid film was rehydrated by vortexing with 5 mL of the internal solution for 5 minutes before brief sonication to ensure no lipid was remaining on the interior wall of the flask. The lipid solution was subjected to nine freeze-thaw cycles by submerging the flask in liquid N_2 and lukewarm water, followed by allowing the solution to rest for 30 minutes. Every 1 mL of the lipid solution was then extruded 27 times through a 200 nm polycarbonate membrane to form unilamellar vesicles. The vesicles were then dialysed against the external solution overnight to remove unencapsulated NaCl. The vesicles were then diluted to 10 mL with the external solution to obtain a stock solution of lipid.

For preparation of POPC vesicles at pH 4.20, the procedure is largely the same. Internal and external solutions are buffered with a citrate buffer to pH 4.20 (5 mM) instead of sodium phosphate. The dialysis of the lipid vesicles to remove unencapsulated NaCl lasts for 2 hours, as opposed to overnight.

Cl^-/NO_3^- exchange assays

In a glass vial, an aliquot of the vesicle solution was diluted to 5 mL using the external solution to obtain a solution of 0.5 mM lipid. A micro PTFE stirring bar was added to the vial and set to

stir at a moderate rate. The chloride ion selective electrode (ISE) was calibrated against standard solution of NaCl before using the ISE to monitor Cl^- efflux. The readings from the electrode reader were allowed to stabilise before initiating the experiment. A negative control using DMSO was added to the lipid solution as to ensure that the vesicles displayed no leakage. At t=0, a DMSO solution of the receptor was added to give a 5 mol % (concentration of the receptor with respect to the lipid) solution. The electrode reader was set to record the mV at 5 second intervals. At t=300, a solution of Triton X-100 (11 wt% in H_2O:DMSO 7:1 *v:v*) was added to lyse the vesicles to determine 100% Cl- efflux. Experiments were each repeated in triplicate, and all traces are the average of three trials.

Computational methods:

Geometry Optimisations

All electronic structure calculations were carried out using the Gaussian 09 (revision E.01)[4] and ORCA (version 4.2.1) program packages.[5] Unconstrained optimizations of ground-state geometries and subsequent analytical frequency calculations were carried out at DFT level using the hybrid meta exchange-correlation M06-2X functional[6] in conjunction with Pople's 6-31+G(d) basis set on all atoms except iodine.[7] The Stuttgart-Dresden SDD effective core potential and associate basis sets were chosen to describe iodine,[8] with an added polarization function (ζ_d = 0.289).[9] An ultrafine integration grid, corresponding to a pruned grid of 99 radial shells and 590 angular points per shell, was used for all calculations. All stationary points were confirmed to be minima by the absence of imaginary modes in their vibrational spectra. Thermal and entropic corrections to the SCF energies (T = 298.15 K and p = 1 atm) were also extracted from the vibrational gas phase calculations. Effects due to the presence of solvent were included by means of a polarizable continuum model in the integral equation formalism variant (IEF-PCM),[10] with dielectric constant and related solvent parameters corresponding to those of dimethylsulfoxide (ϵ = 46.8). Non-electrostatic terms to solvation were calculated by invoking the SMD option.[11] To this end, all geometries were re-optimised in solution phase. The free energies of solvation (at fixed concentrations) for each compound were then obtained from the electronic energy difference of the species optimised in solution and gas phase:

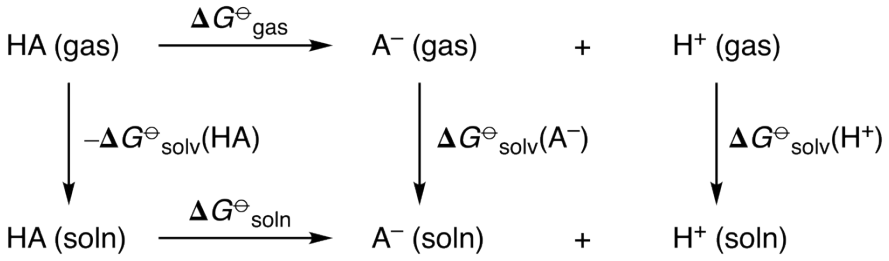
$$\Delta G^{\ominus}_{solv} = E_{SCRF}(\boldsymbol{R}_s) - E_{SCF}(\boldsymbol{R}_g)$$

The "⊖" superscript indicates that the quantities are calculated with respect to standard states of 1 mol L^{-1} (applying a correction of 1.9 kcal mol^{-1}). The variables $\boldsymbol{R}_g$ and $\boldsymbol{R}_s$ imply dependence of the energy on the gas phase and solution phase optimized geometries, respectively. High-level gas phase calculations were carried out at the DLPNO-CCSD(T) level of theory[12] as implemented in ORCA, by means of single-point calculations on the DFT-optimised geometries. Automatic basis set extrapolation[13] (involving cardinal numbers n = 3 and 4 within the def2-*n*ZVP basis set family)[14] was used to converge both HF and correlation energies to the complete basis set limit. The RIJCOSX approximation was used to speed up integral solvation, in conjunction with the autoaux option to construct auxiliary basis sets for Coulomb, exchange and correlation calculations.[15]

Calculations of pK_A values

All pK_a values were calculated following literature procedures[16] and using the direct method via the thermodynamic cycle depicted in Scheme S1. A proton solvation free energy of –273.30 kcal mol^{-1} in DMSO was employed.[17]

Scheme S1:



$$\Delta G^{\ominus}_{soln} = \Delta G^{\ominus}_{gas} + \Delta G^{\ominus}_{solv}(H^+) + \Delta G^{\ominus}_{solv}(A^-) - \Delta G^{\ominus}_{solv}(HA)$$

$$pK_a(HA) = \Delta G^{\ominus}_{soln} / RT\ln(10)$$

Metadynamics Simulations

After a preliminary minimization, receptor **1** was subjected to well-tempered metadynamics simulations,[18] utilizing the ABIN (version 1.1)[19] molecular dynamics software in conjunction with the PLUMED (version 2.6.0) plugin.[20] Forces and energies were obtained externally by interfacing to the xtb 6.1 code[21] (invoking the GBSA model for water solvent). These simulations employed a Nosé-Hoover[22] thermostat at a temperature of 298.15 K, using a time step of 20 au (~0.5 fs). For each system, two collective variables (CV1 and CV2) were defined as torsional angles (see Figure 3 in for definition). After a first trial phase where the simulation parameters were tuned properly, the Gaussian width for both CVs was set to 0.35 radians, spawned every 500 steps. A Gaussian height of 1.2 kJ mol^{-1} and a bias factor of 6.0 was used in all cases. In order to sample the conformational space efficiently, 40 multiple walkers were run in parallel during the simulation. The deposited bias is shared along all replicas (disk-based sharing) so that the history-dependent potential depends on the full history. The free energy surfaces (FESs) were obtained from the combined bias potential from all trajectories as calculated with respect to the two CVs. General searches of the conformations space for all receptors utilised the automated crest routine as implemented in xtb 6.1.[23]

Spectroscopic Characterisation Data:

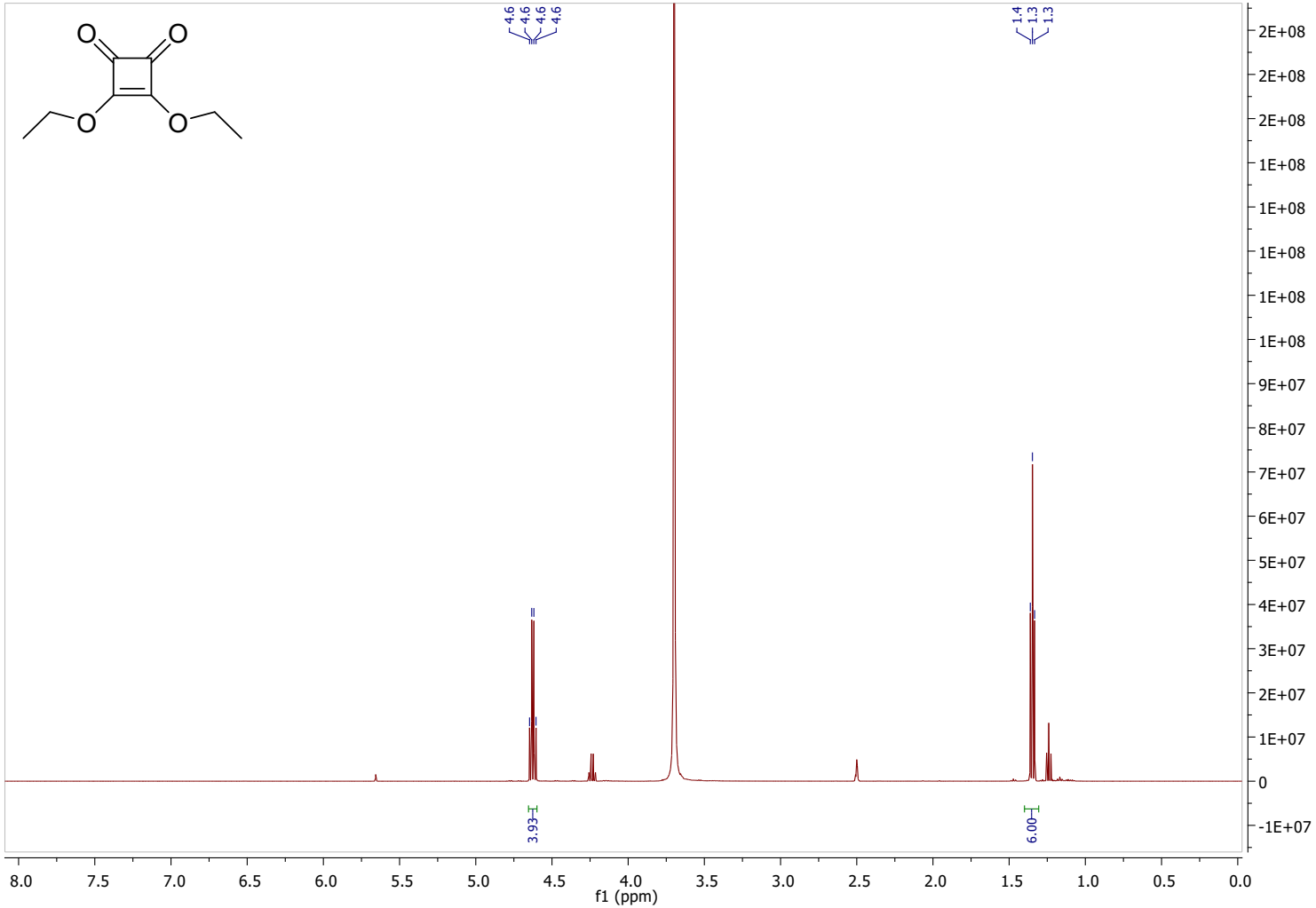


Figure S1. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***1.***

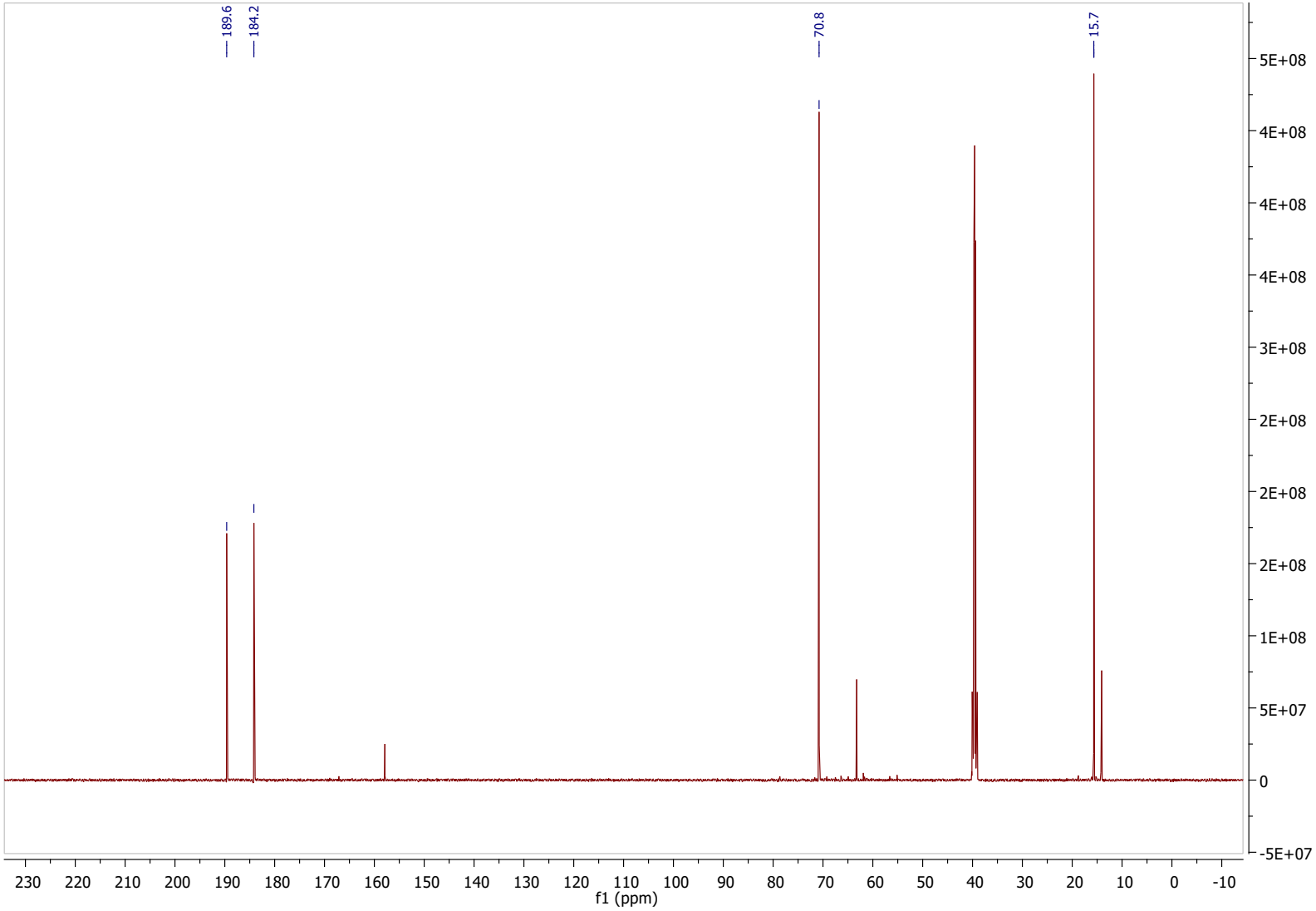


Figure S2. *^{13}C NMR (DMSO-d_6, 500 MHz) spectrum of* ***9****.*

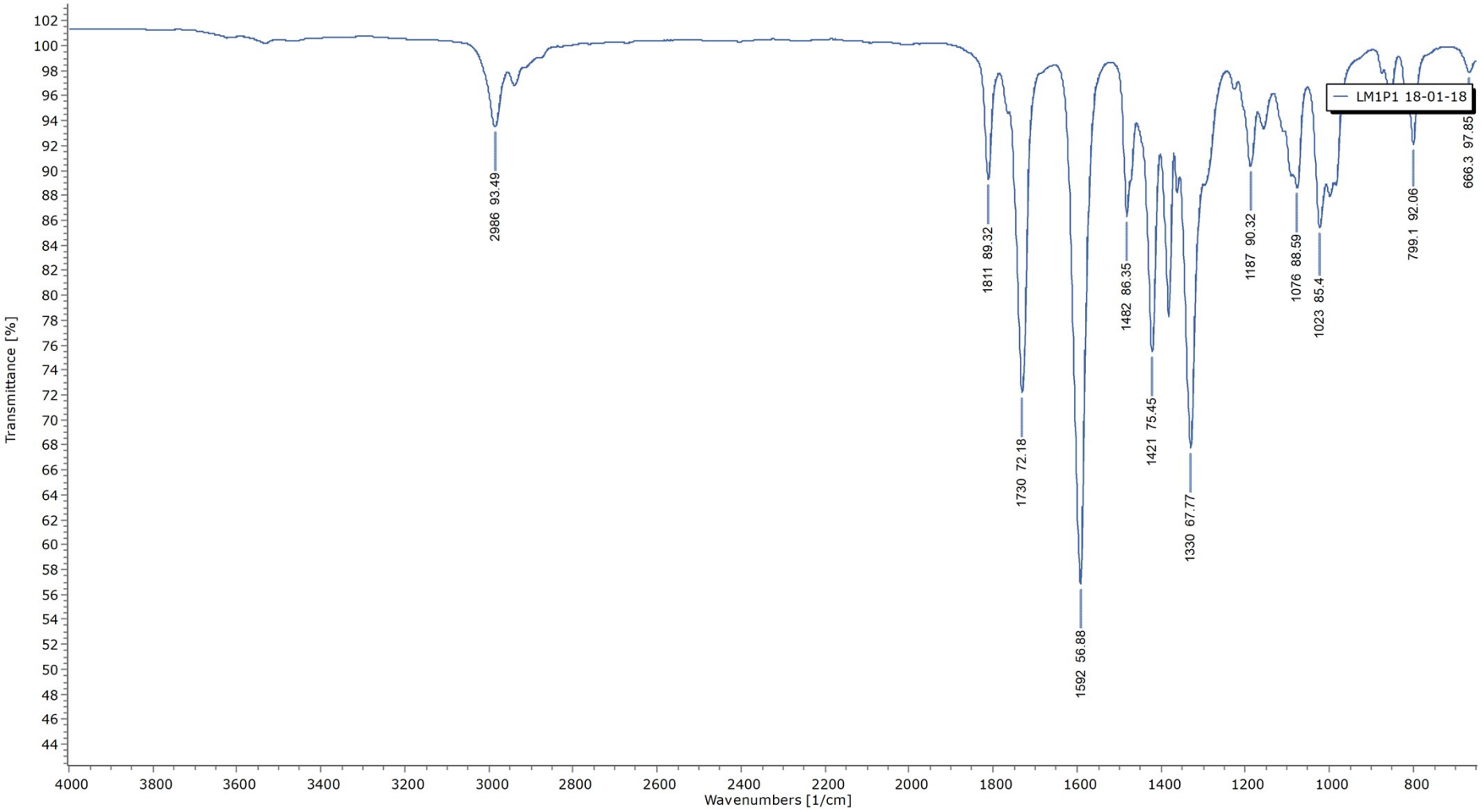
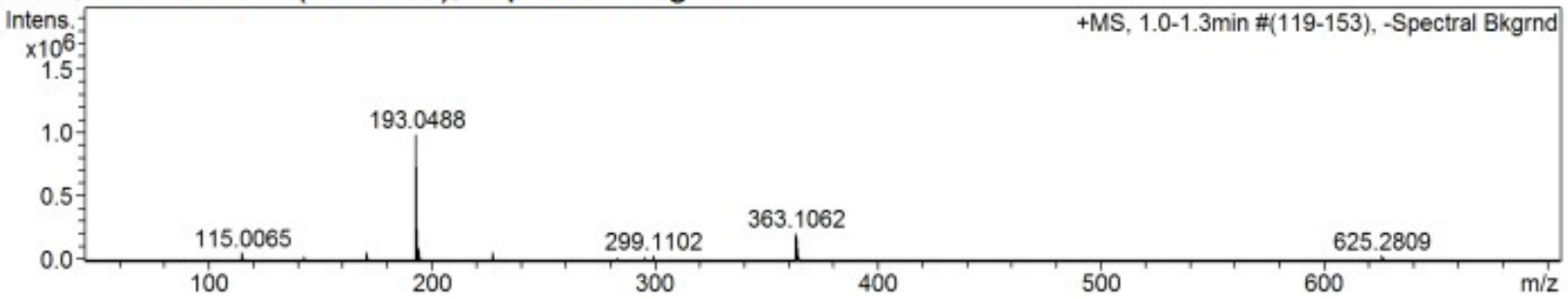


Figure S3. *IR spectrum of* ***9****.*

+MS, 1.0-1.3min #(119-153), -Spectral Bkgrnd



#	m/z	I	I %	Area	S/N
1	115.0065	55950	5.7	1041	3998.3
2	171.0653	60124	6.1	1824	1852.8
3	193.0488	987338	100.0	39236	18352.4
4	194.0501	91896	9.3	3202	1677.7
5	227.0885	61454	6.2	2490	1909.0
6	295.1497	32601	3.3	1674	1013.4
7	299.1102	35754	3.6	1787	1150.1
8	363.1062	212150	21.5	13058	4895.7
9	364.1089	34991	3.5	2097	795.5
10	625.2809	36818	3.7	3708	3178.1

Generate Molecular Formula Parameters

Charge	Tolerance	SearchRadius	H/C Ratio min.	H/C Ratio max.	Electron Conf.	Nitrogen Rule	sigma limit
positive	50 ppm	0.05 m/z	0	3	both	true	0.05

Expected Formula C8H10O4 **Adduct(s):** H, Na

#	meas. m/z	theo. m/z	Err[ppm]	Sigma	Formula
1	171.0653	171.0652	0.70	0.0134	C 8 H 11 O 4
1	193.0488	193.0471	8.80	0.0040	C 8 H 10 Na 1 O 4

Note: Sigma fits < 0.05 indicates high probability of correct MF.

Figure S4. *HRMS of* ***9****.*

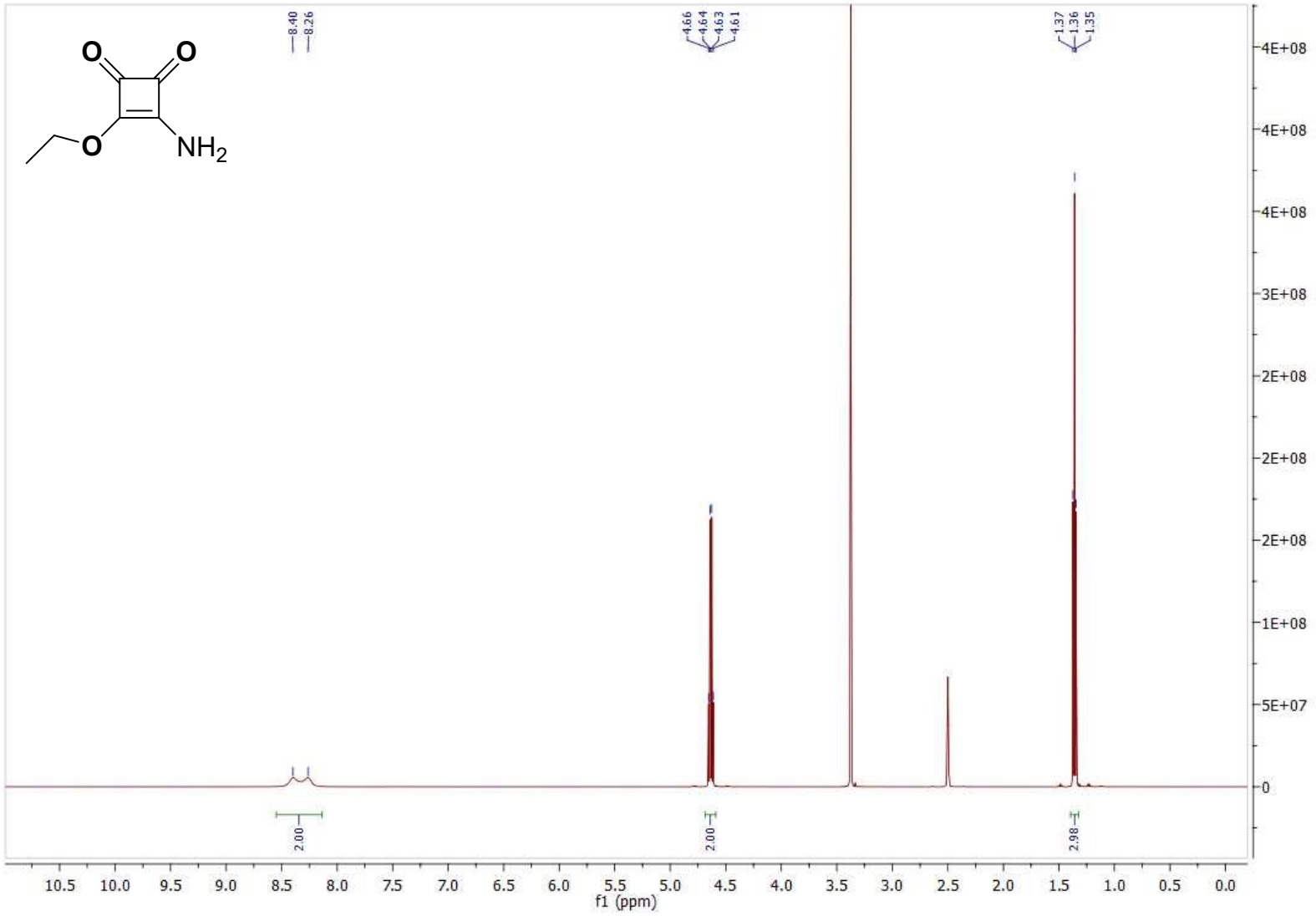


Figure S5. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***10****.*

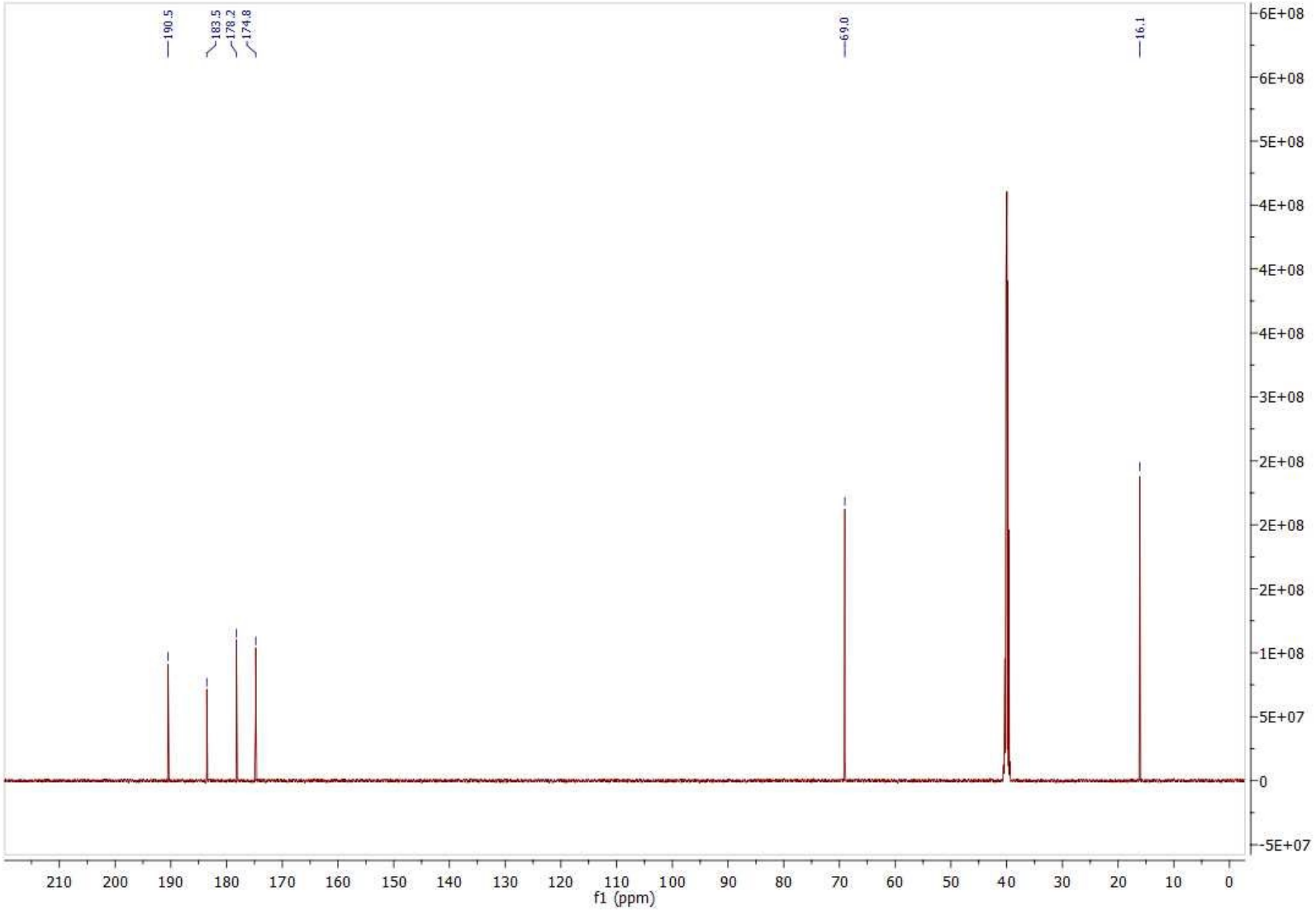


Figure S6. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***10****.*

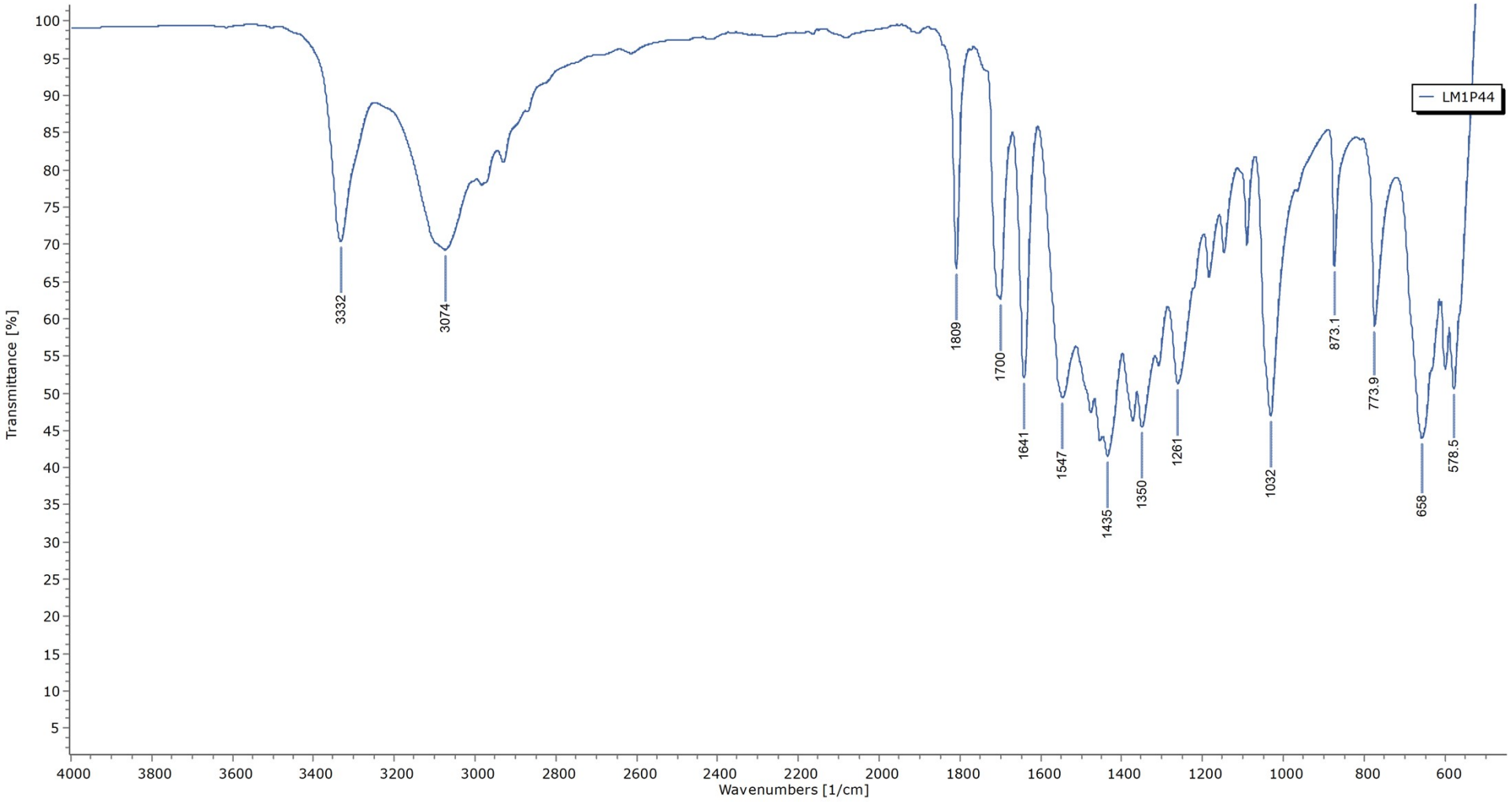
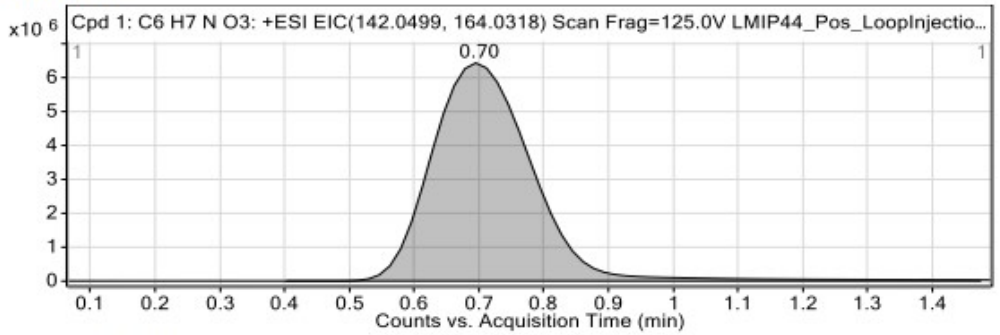


Figure S7. *IR spectrum of* ***2.18***

Compounds



Integration Peak List

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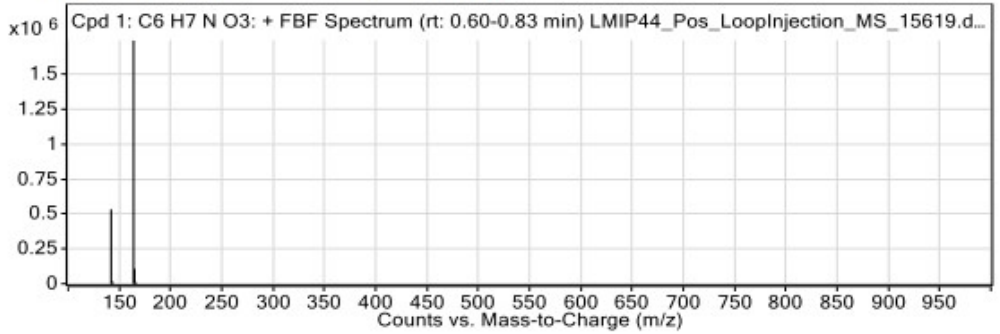

Peak List

m/z	z	Abund	Formula	Ion
142.0501	1	533324.88	C6H7NO3	(M+H)+
143.0343	1	19225.4	C6H7NO3	(M+H)+
144.033	1	2734.74	C6H7NO3	(M+H)+
164.032	1	1746564	C6H7NO3	(M+Na)+
165.0353	1	107480.85	C6H7NO3	(M+Na)+
166.0368	1	12796.33	C6H7NO3	(M+Na)+

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Figure S8. *HRMS of* ***10****.*

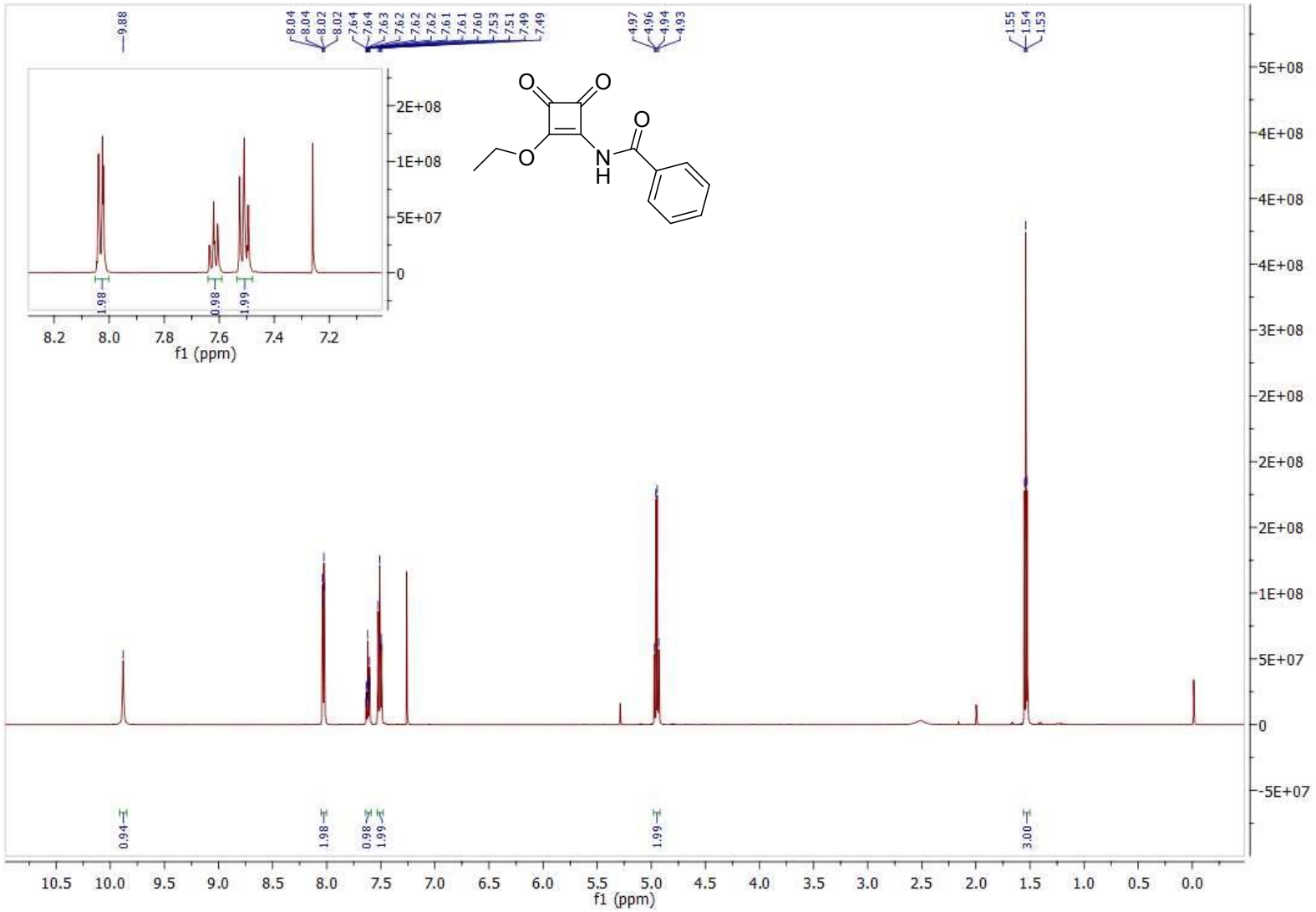


Figure S9. *^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of* ***11****.*

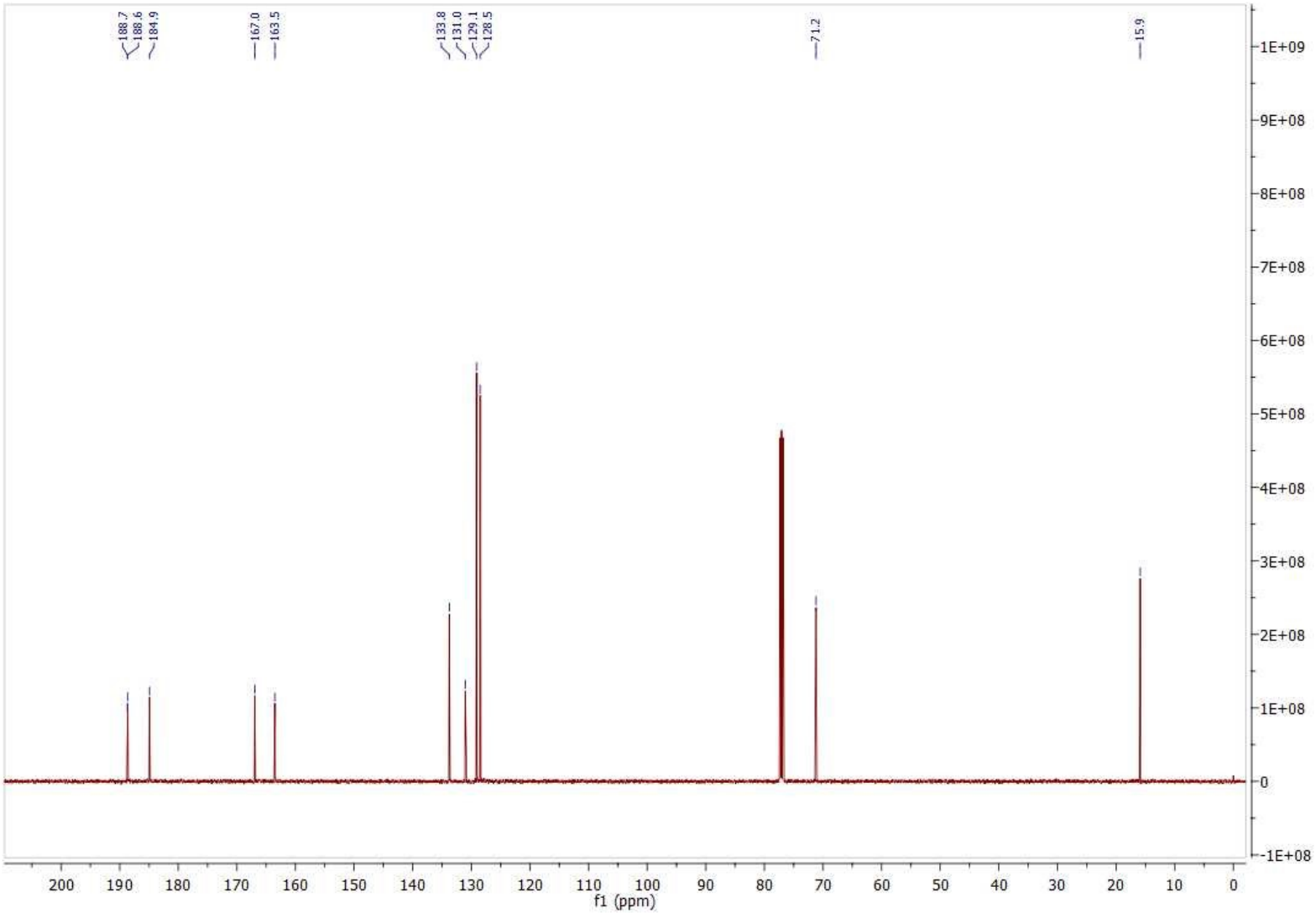


Figure S10. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***11****.*

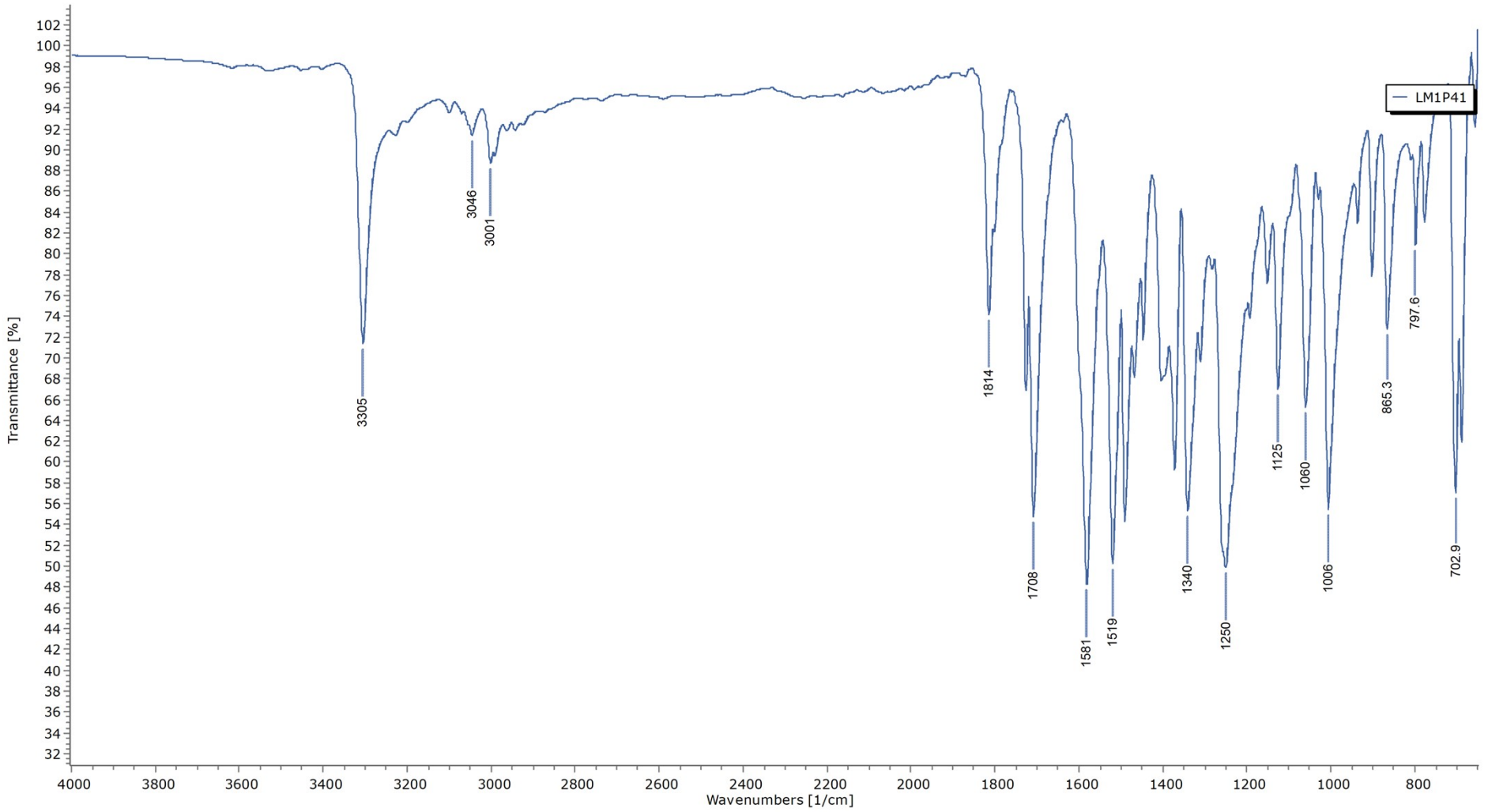
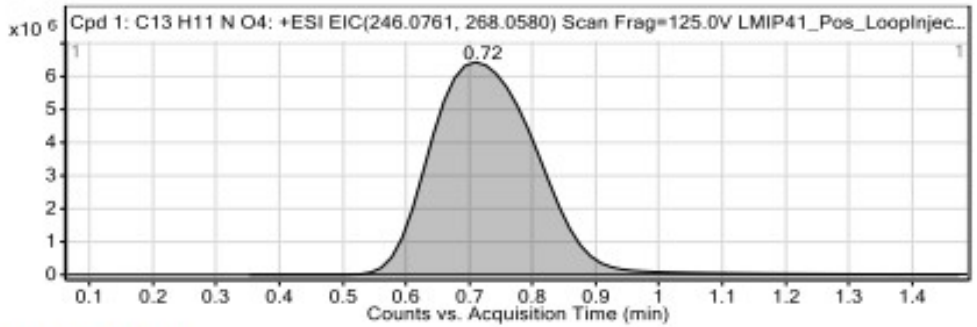


Figure S11. *IR spectrum of* ***11.***

Compounds



Integration Peak List

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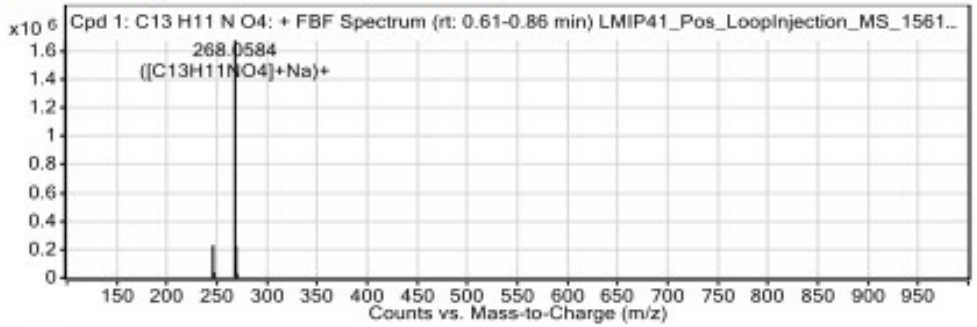

Peak List

m/z	z	Abund	Formula	Ion
246.0764	1	230198.02	C13H11NO4	(M+H)+
247.0794	1	36925.43	C13H11NO4	(M+H)+
248.081	1	4828.54	C13H11NO4	(M+H)+
268.0584	1	1675168.63	C13H11NO4	(M+Na)+
269.0617	1	222764.42	C13H11NO4	(M+Na)+
270.0638	1	29288.15	C13H11NO4	(M+Na)+
271.0669	1	3066.31	C13H11NO4	(M+Na)+

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Figure S12. *HRMS of* ***11****.*

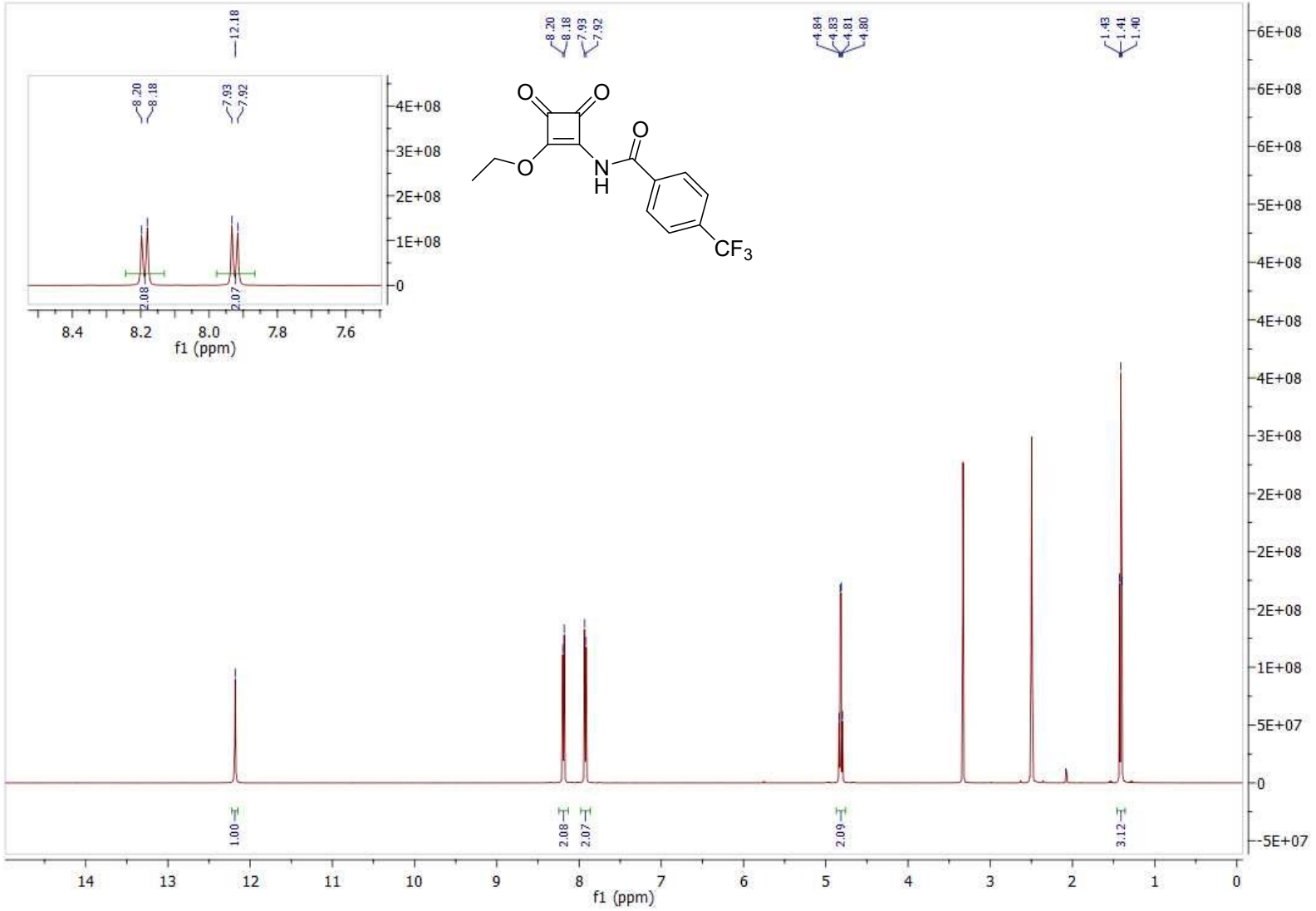


Figure S13. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***12****.*

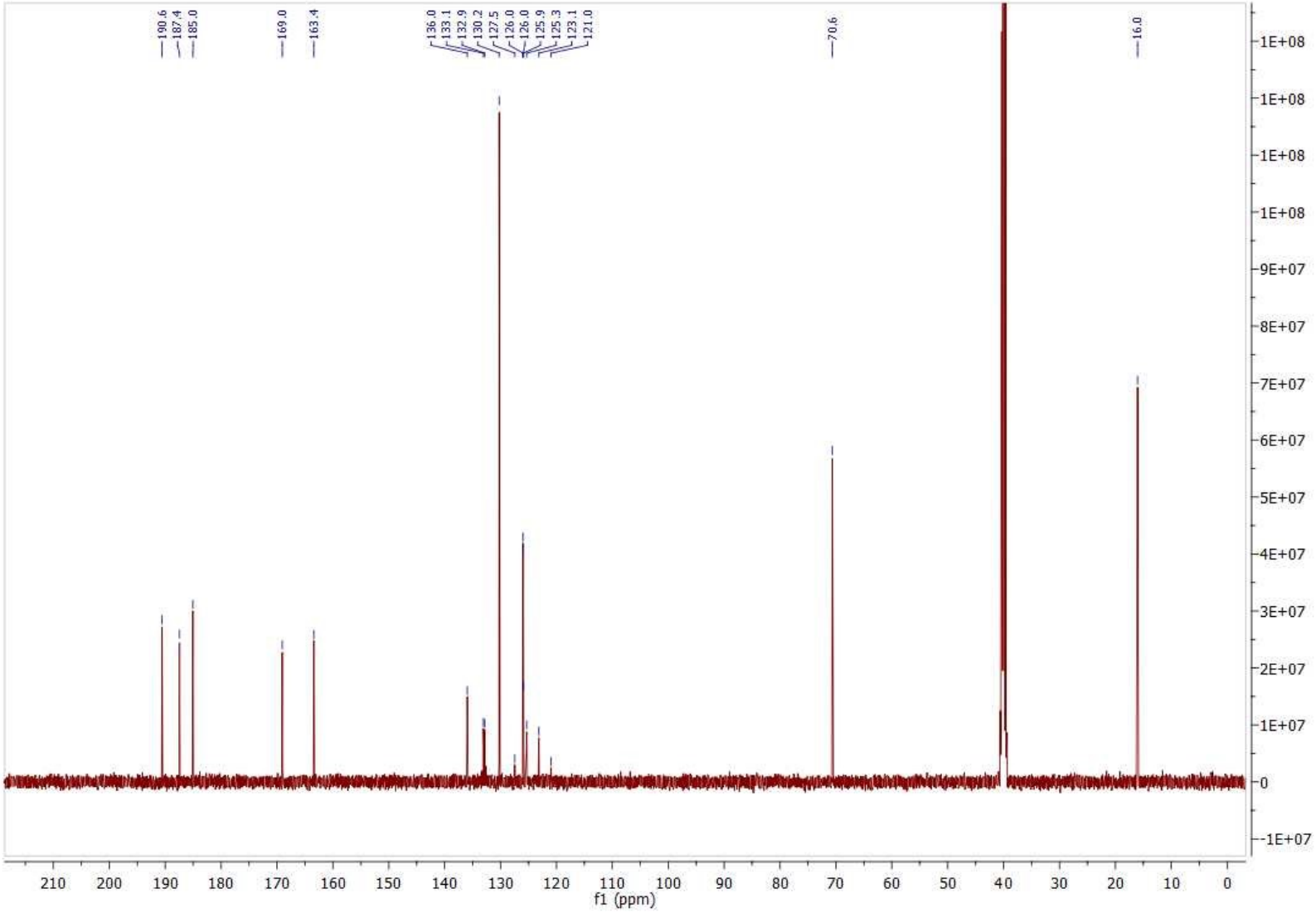


Figure S14. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***12****.*

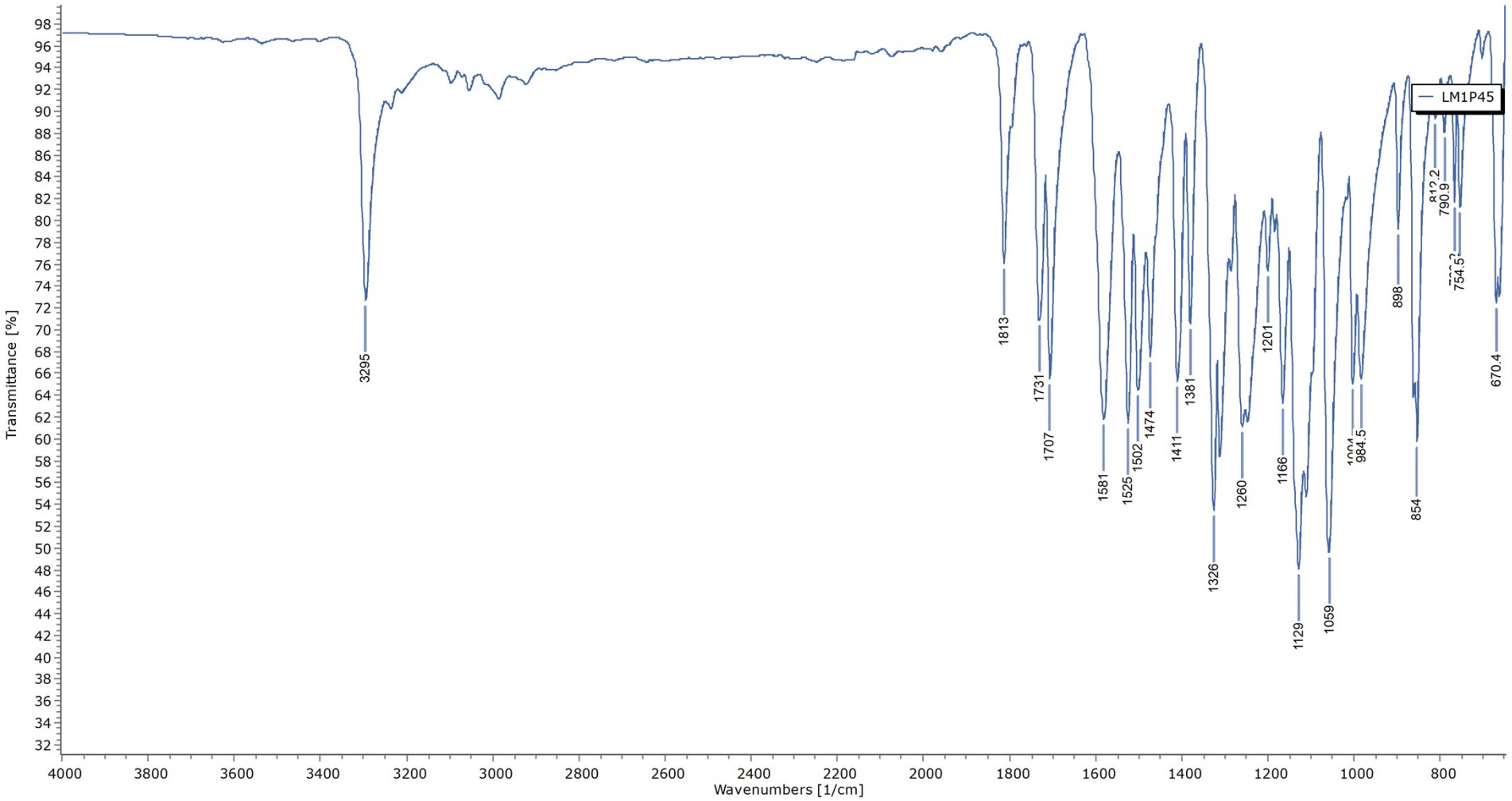
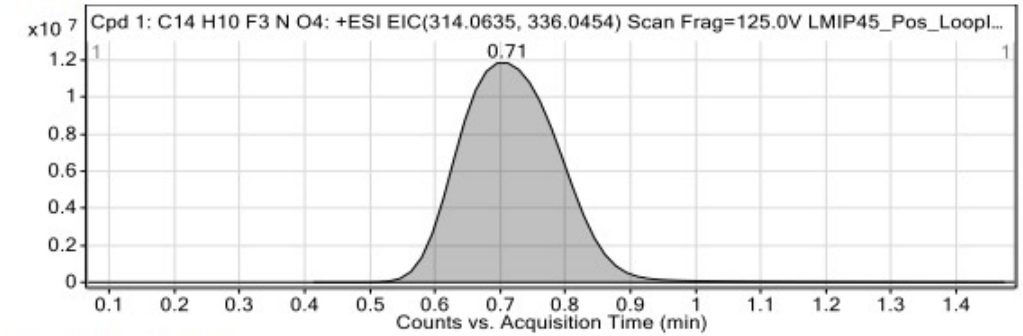


Figure S15. *IR spectrum of* ***12.***

Compounds



Integration Peak List

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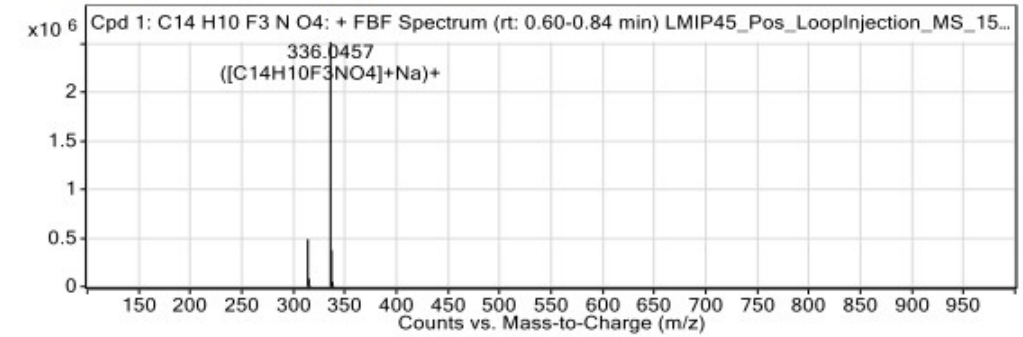


Peak List

m/z	z	Abund	Formula	Ion
314.0637	1	486639.28	C14H10F3NO4	(M+H)+
315.0676	1	80786.87	C14H10F3NO4	(M+H)+
316.0704	1	9808.21	C14H10F3NO4	(M+H)+
336.0457	1	2520331.75	C14H10F3NO4	(M+Na)+
337.0492	1	374240.66	C14H10F3NO4	(M+Na)+
338.0514	1	46300.03	C14H10F3NO4	(M+Na)+
339.0548	1	4834.05	C14H10F3NO4	(M+Na)+

--- End Of Report ---

Figure S16. *HRMS of* ***12.***

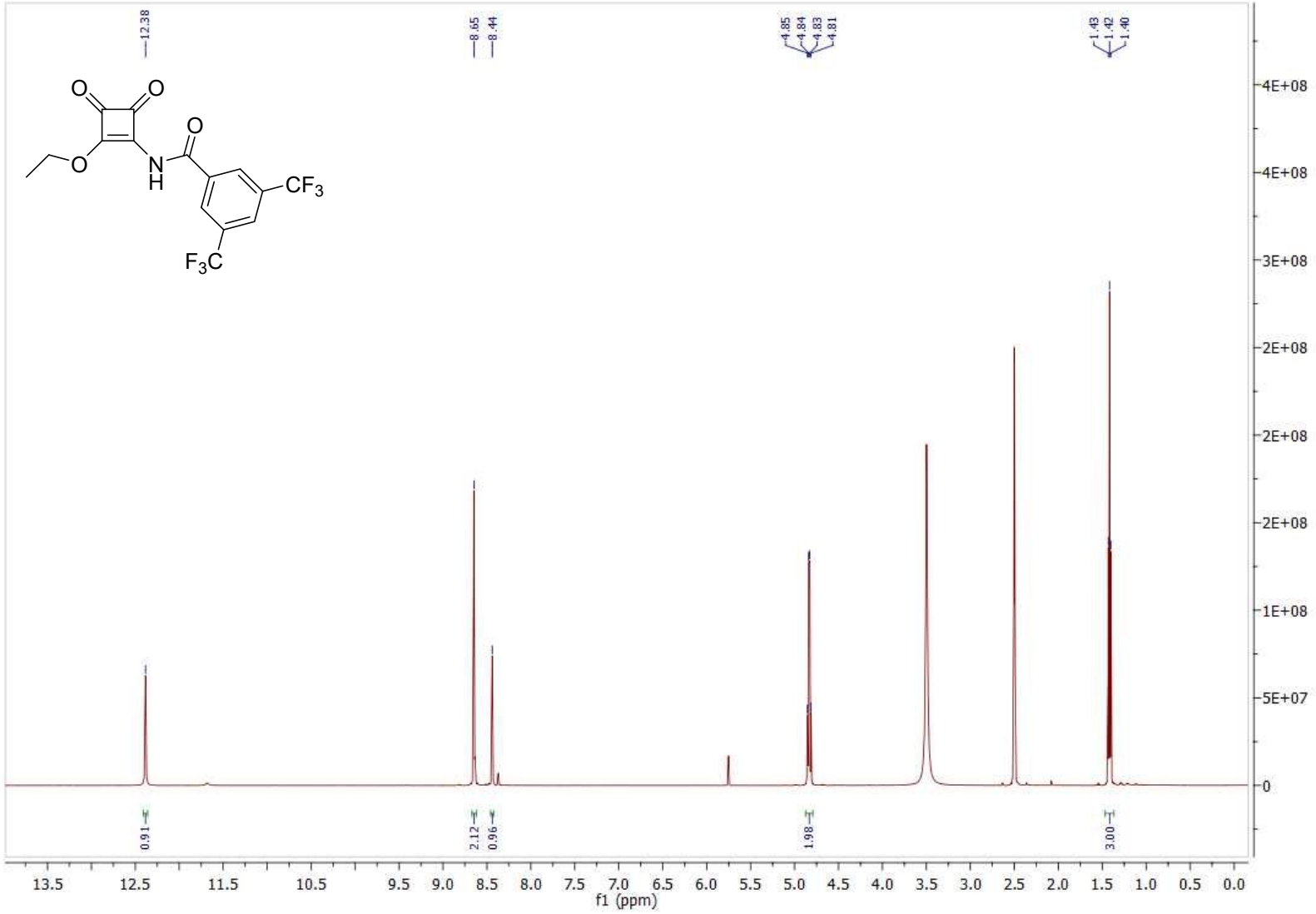


Figure S17. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***13****.*

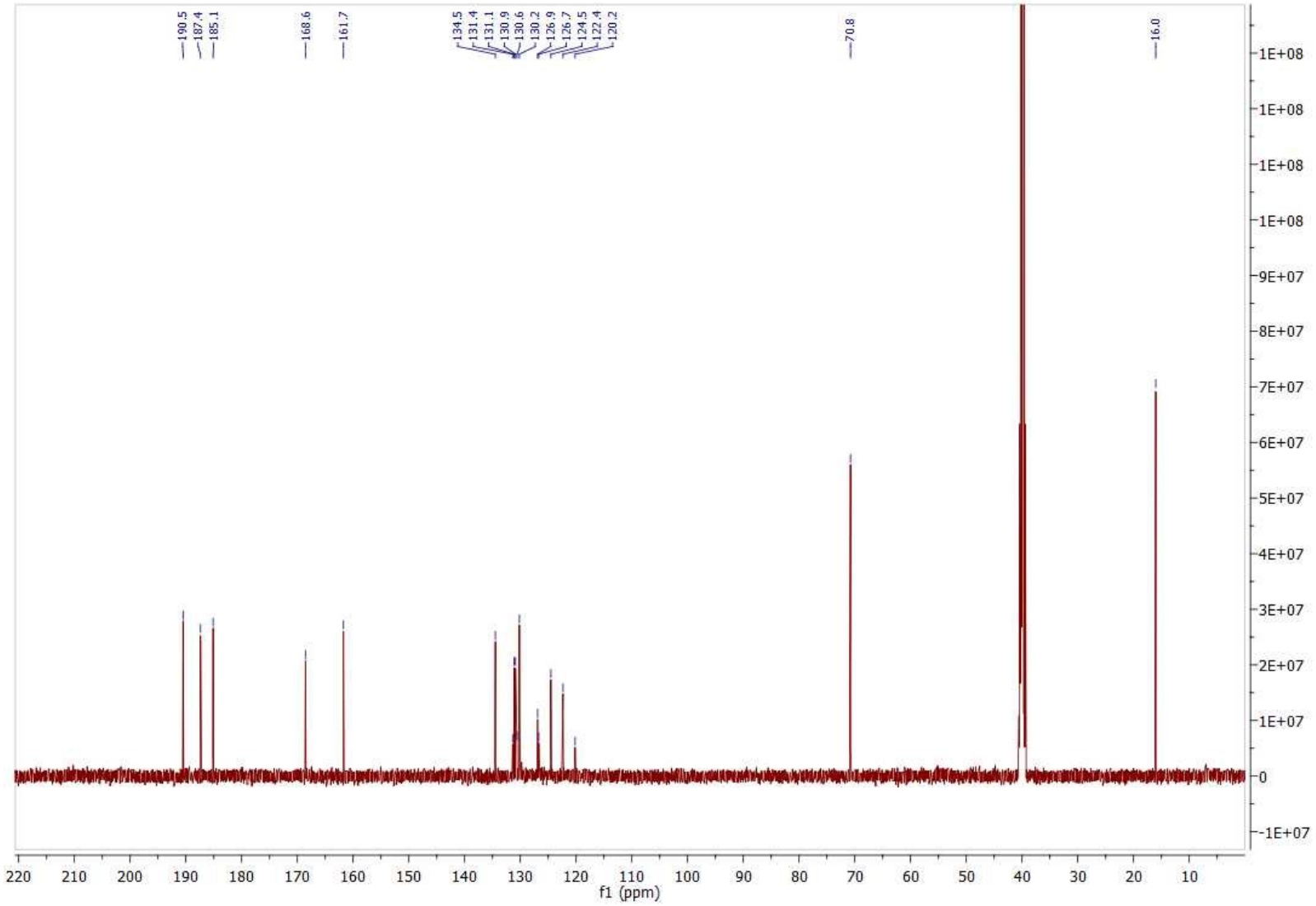


Figure S18. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***13****.*

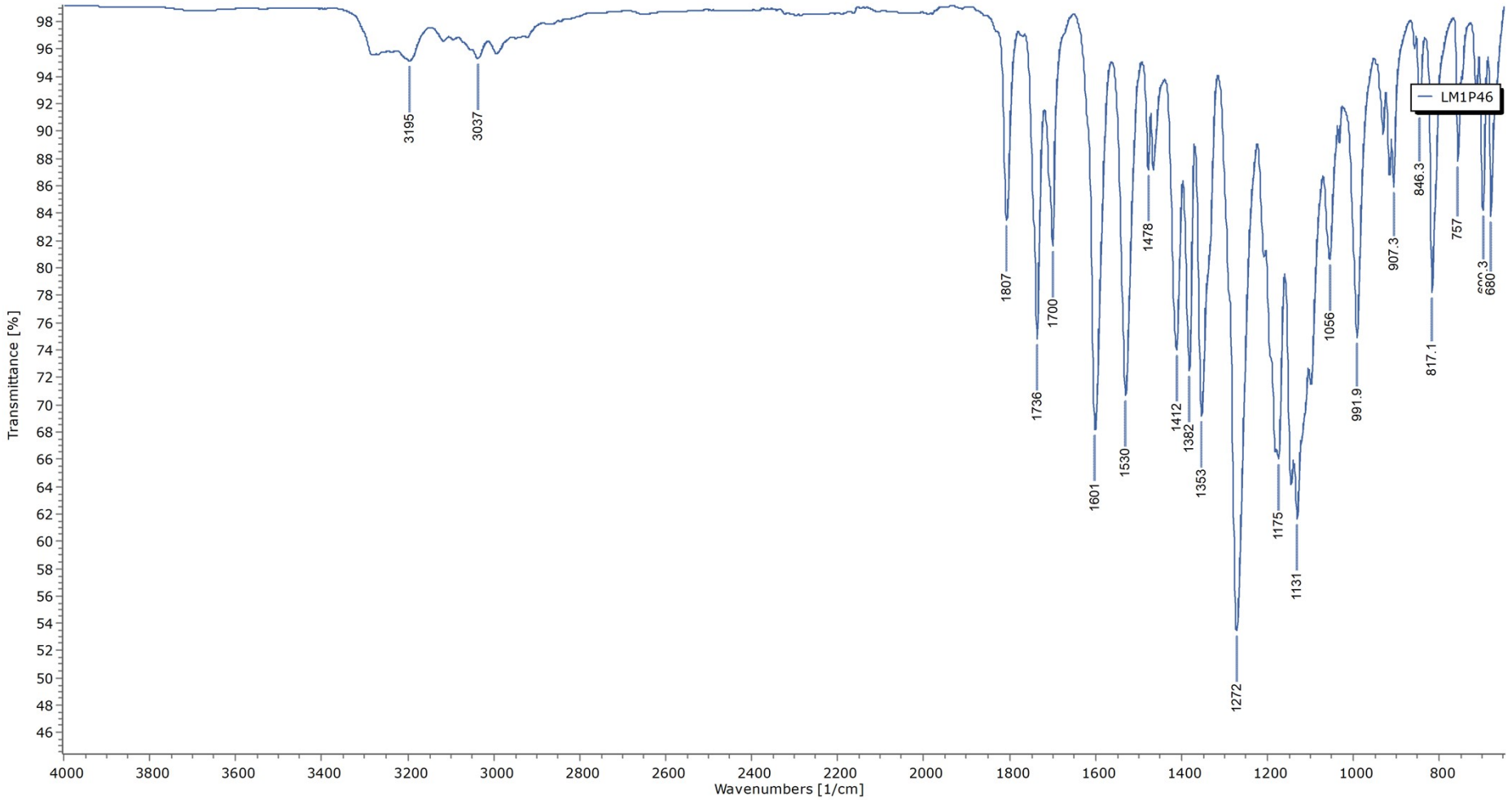
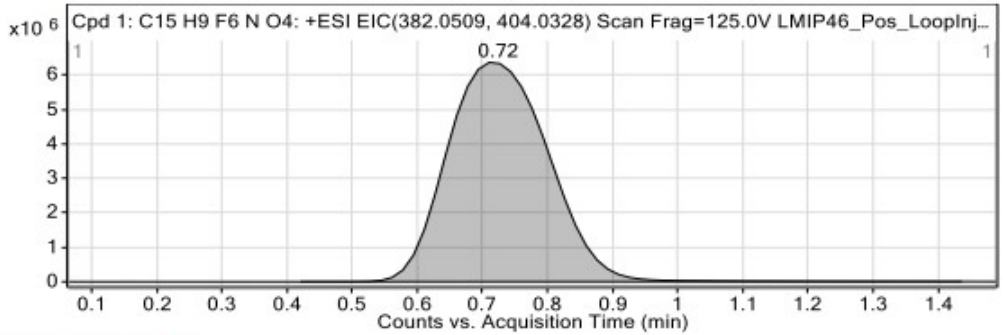


Figure S19. *IR spectrum of* ***13.***

Compounds



Integration Peak List

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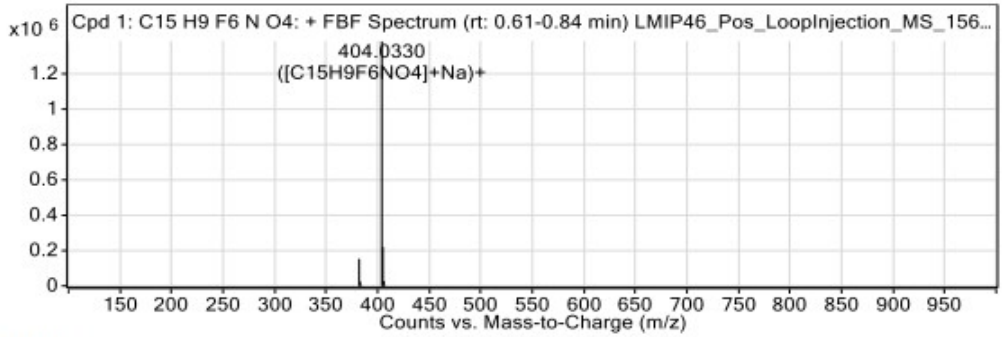

Peak List

m/z	z	Abund	Formula	Ion
382.051	1	153784.44	C15H9F6NO4	(M+H)+
383.0541	1	23695.58	C15H9F6NO4	(M+H)+
384.0563	1	3103.73	C15H9F6NO4	(M+H)+
404.033	1	1386279.25	C15H9F6NO4	(M+Na)+
405.0365	1	220258.97	C15H9F6NO4	(M+Na)+
406.0385	1	27570.79	C15H9F6NO4	(M+Na)+
407.0411	1	2809.82	C15H9F6NO4	(M+Na)+

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Figure S20. *HRMS of* ***13.***

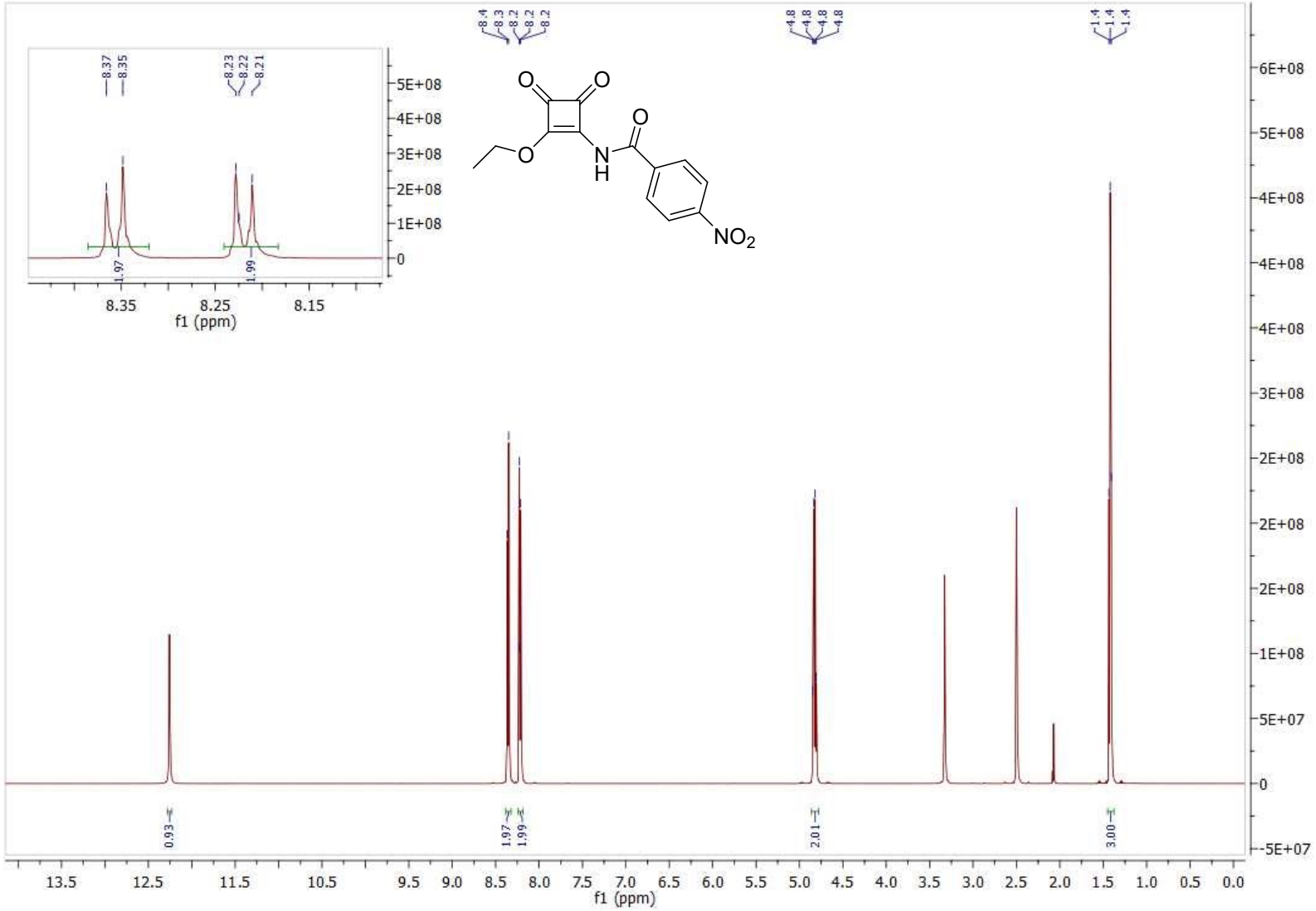


Figure S21. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***14****.*

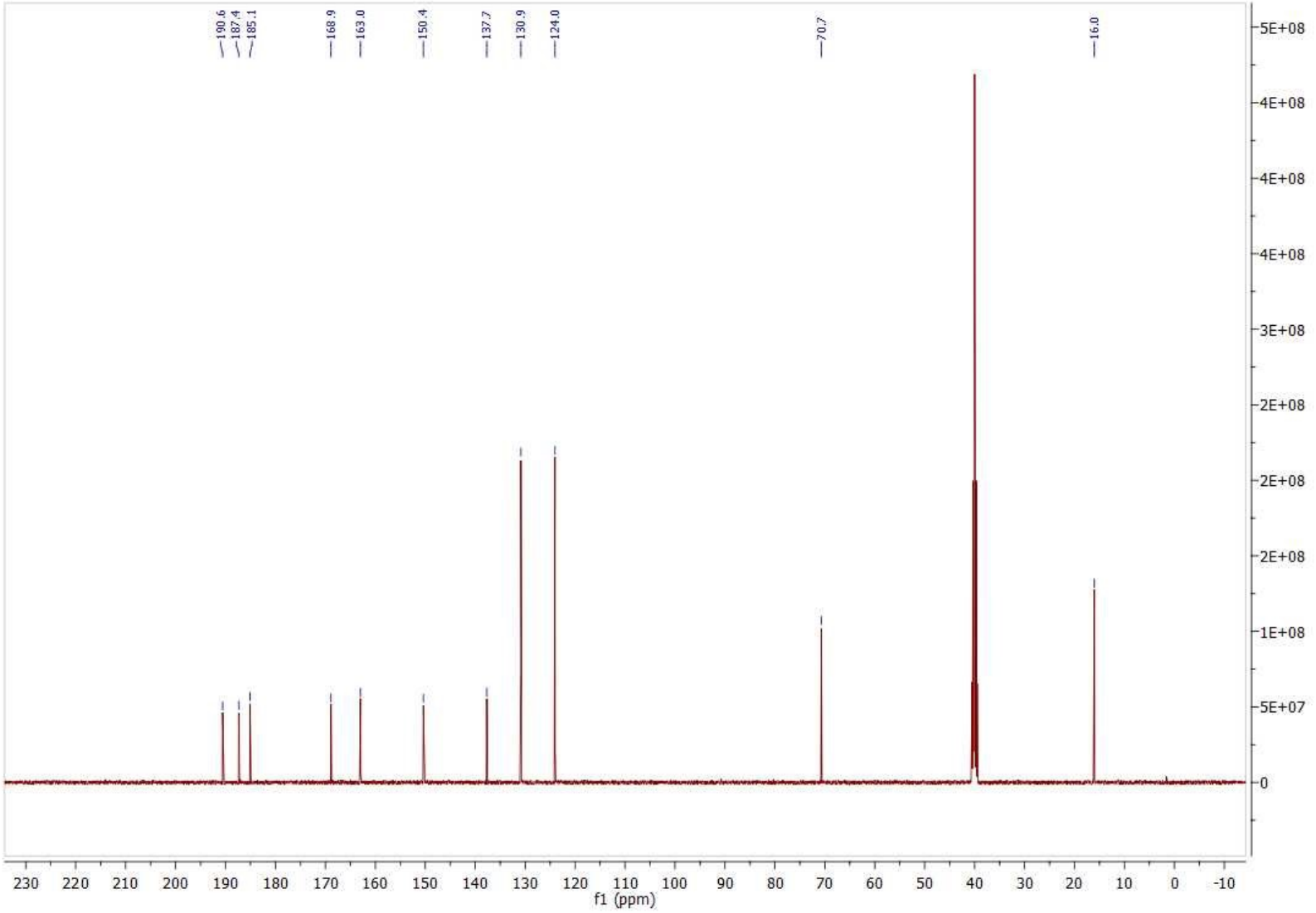


Figure S22. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***14****.*

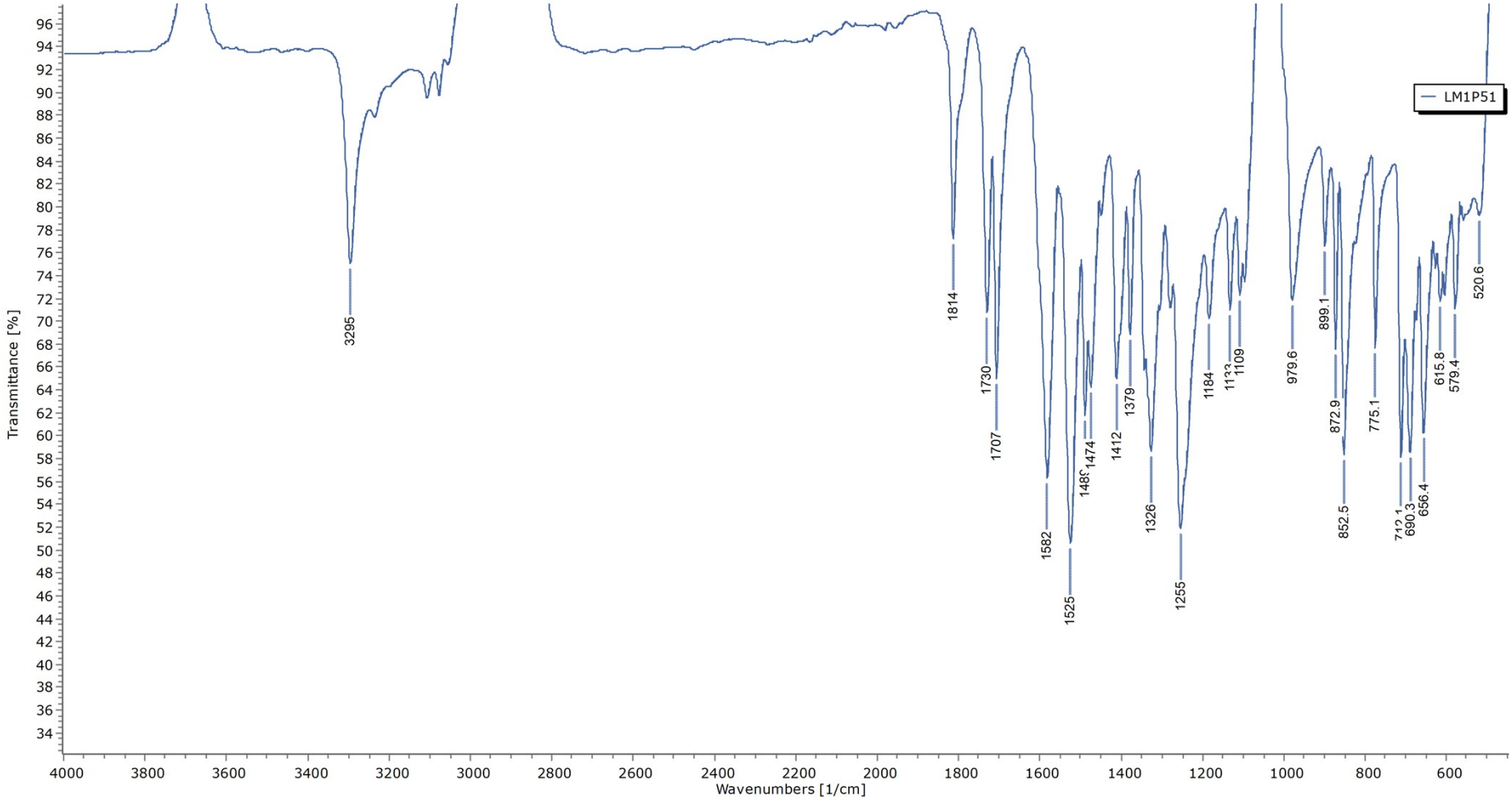
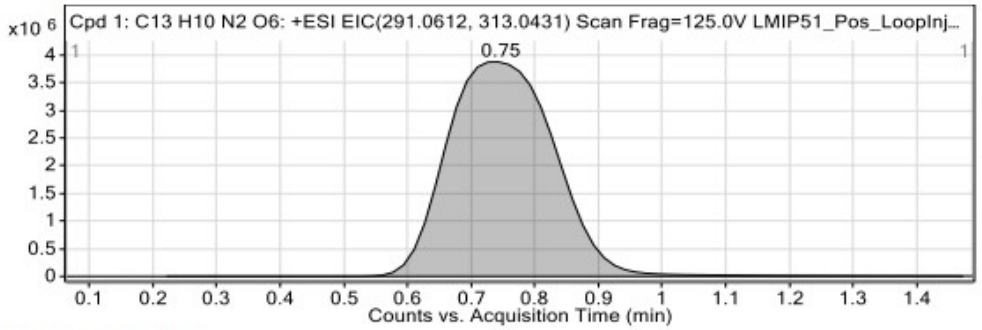


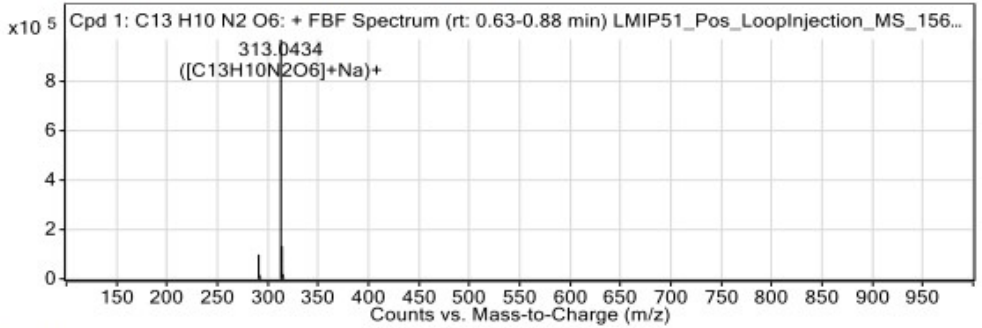
Figure S23. *IR spectrum of* ***14.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.22	0.75	1.47	3822997	46311078



Peak List

m/z	z	Abund	Formula	Ion
291.0613	1	98875.48	C13H10N2O6	(M+H)+
292.0647	1	15112.59	C13H10N2O6	(M+H)+
293.0672	1	2379.04	C13H10N2O6	(M+H)+
313.0434	1	972596.19	C13H10N2O6	(M+Na)+
314.0467	1	133088.45	C13H10N2O6	(M+Na)+
315.049	1	20580.38	C13H10N2O6	(M+Na)+
316.0516	1	2236.74	C13H10N2O6	(M+Na)+

--- End Of Report ---

Figure S24. *HRMS of* ***14.***

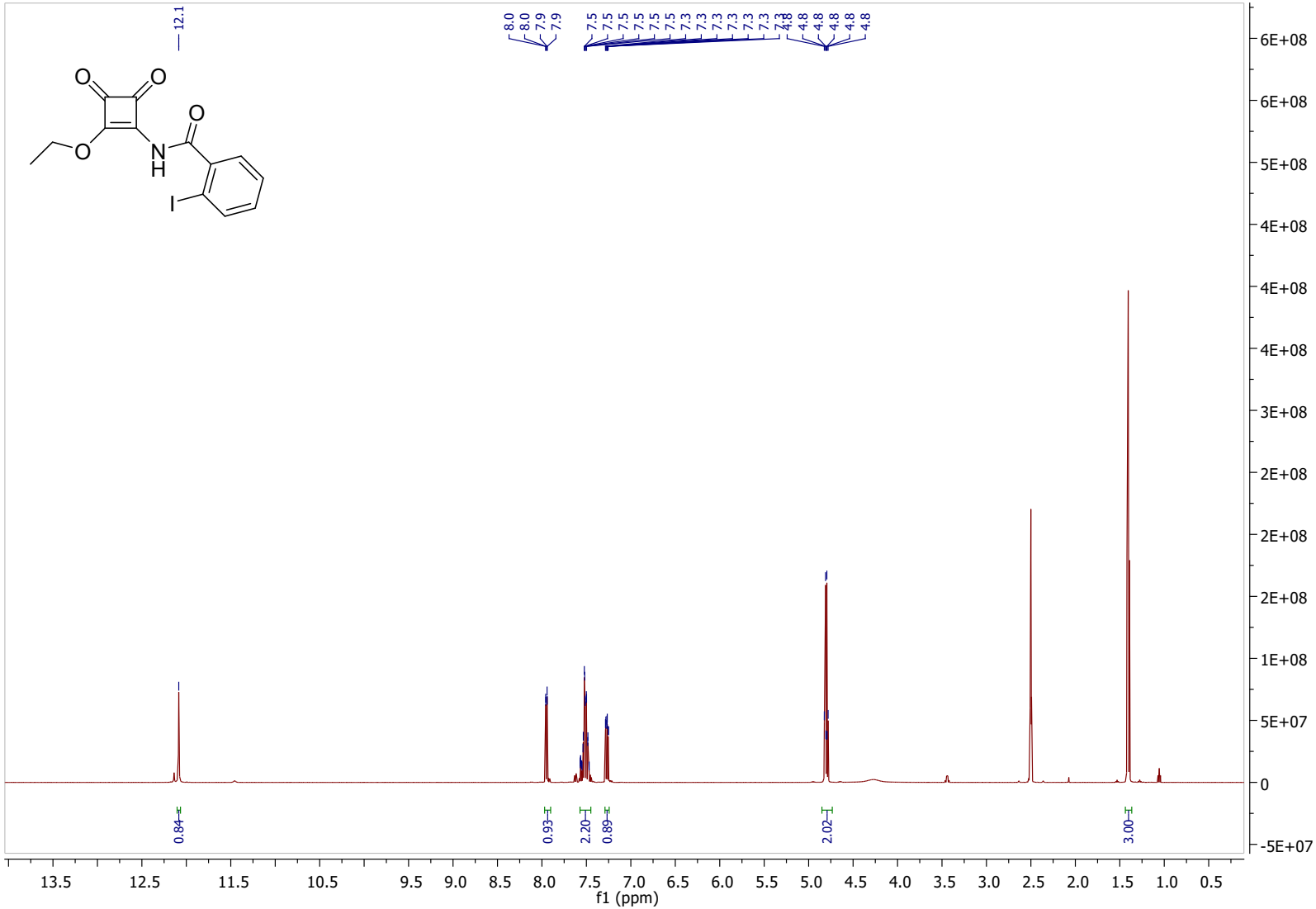


Figure S25. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***15****.*

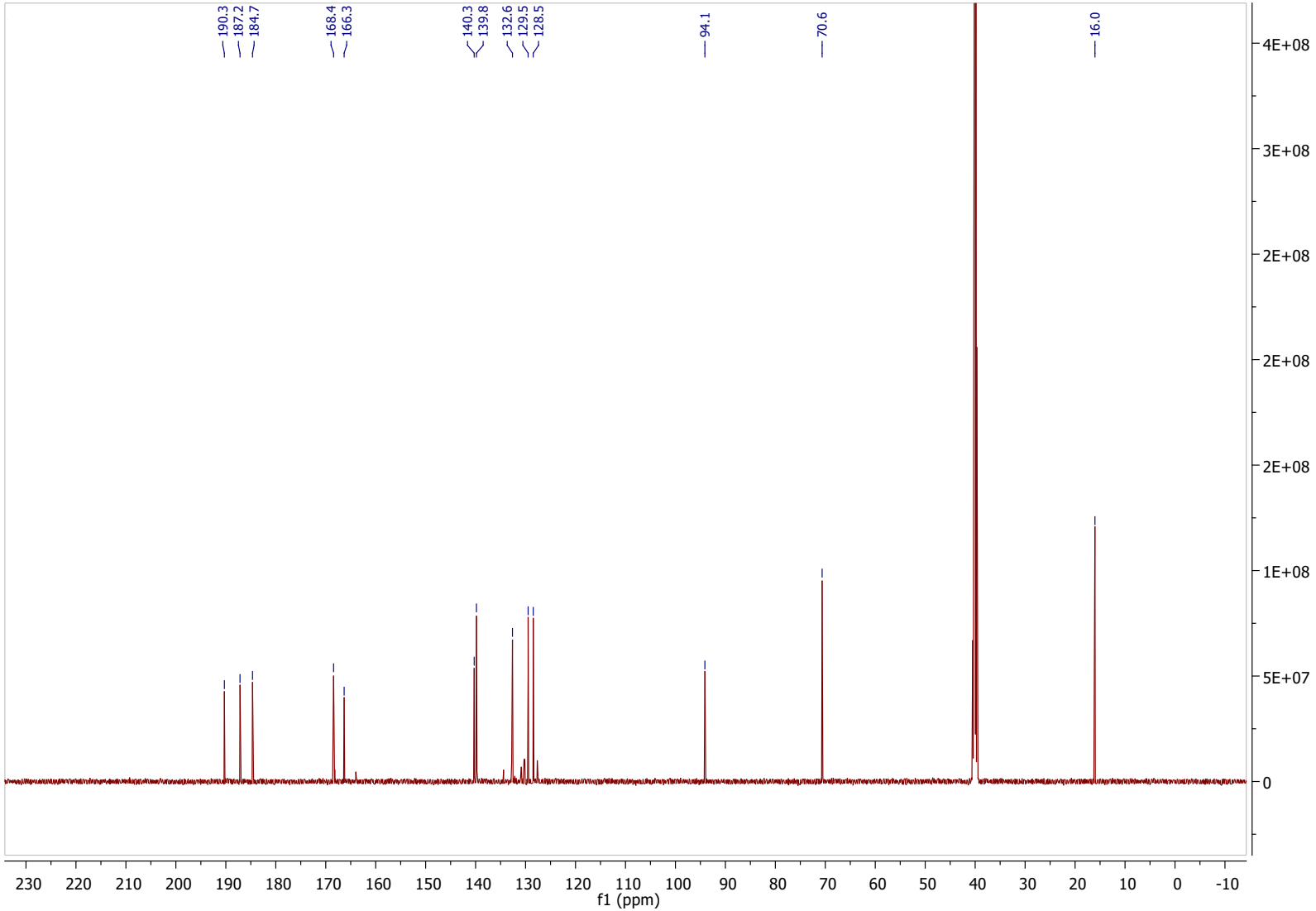


Figure S26. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***15****.*

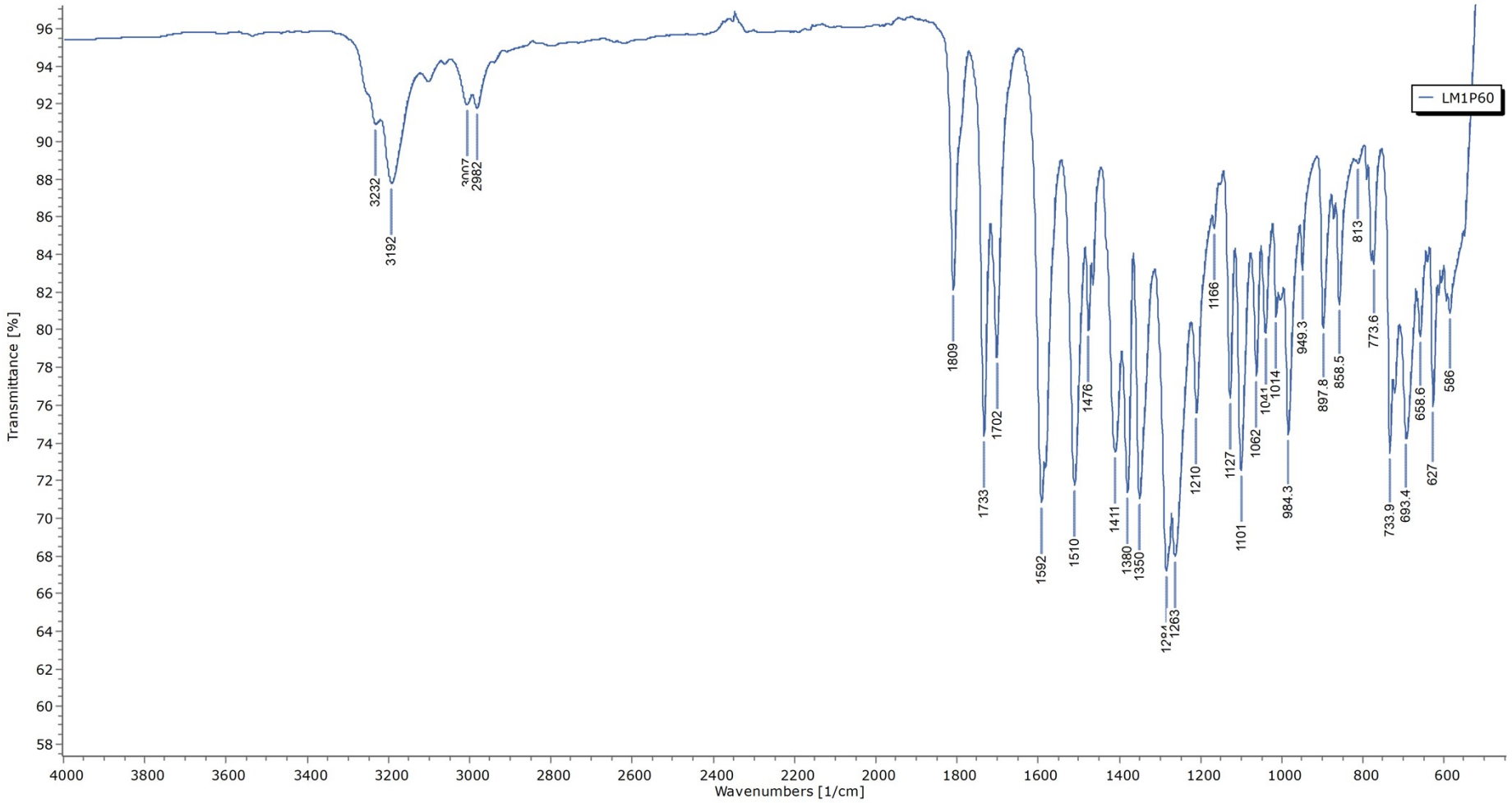
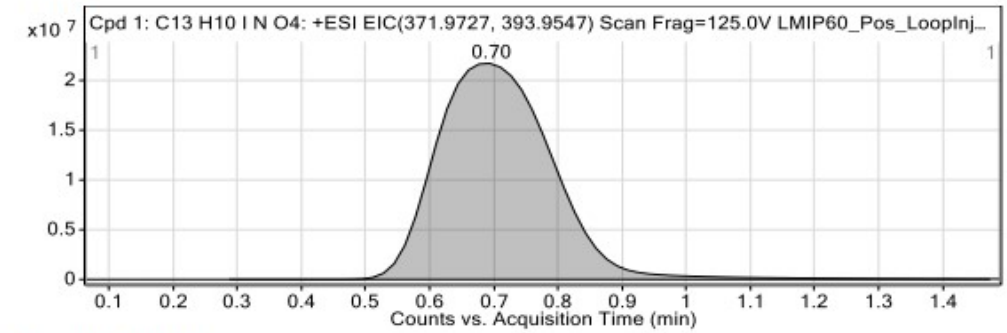


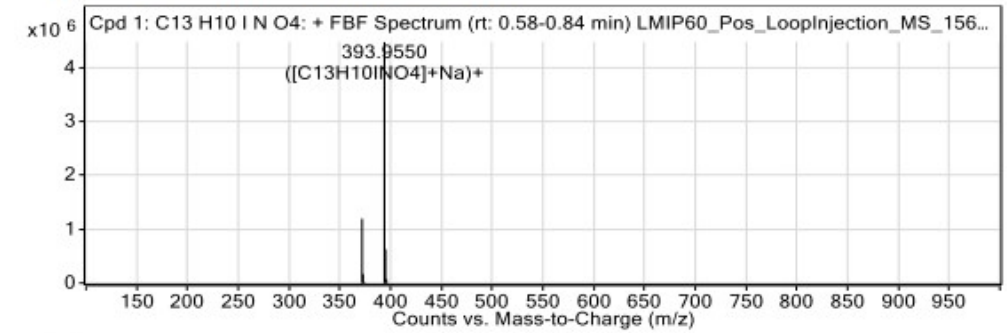
Figure S27. *IR spectrum of* ***15.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.29	0.7	1.47	21498565	273497514



Peak List

m/z	z	Abund	Formula	Ion
371.9728	1	1196103.25	C13H10INO4	(M+H)+
372.9761	1	167462.86	C13H10INO4	(M+H)+
373.9784	1	20403.75	C13H10INO4	(M+H)+
393.955	1	4484876.5	C13H10INO4	(M+Na)+
394.9583	1	630267.38	C13H10INO4	(M+Na)+
395.9603	1	72445.63	C13H10INO4	(M+Na)+
396.9626	1	6382.16	C13H10INO4	(M+Na)+

--- End Of Report ---

Figure S28**. HRMS of **15.

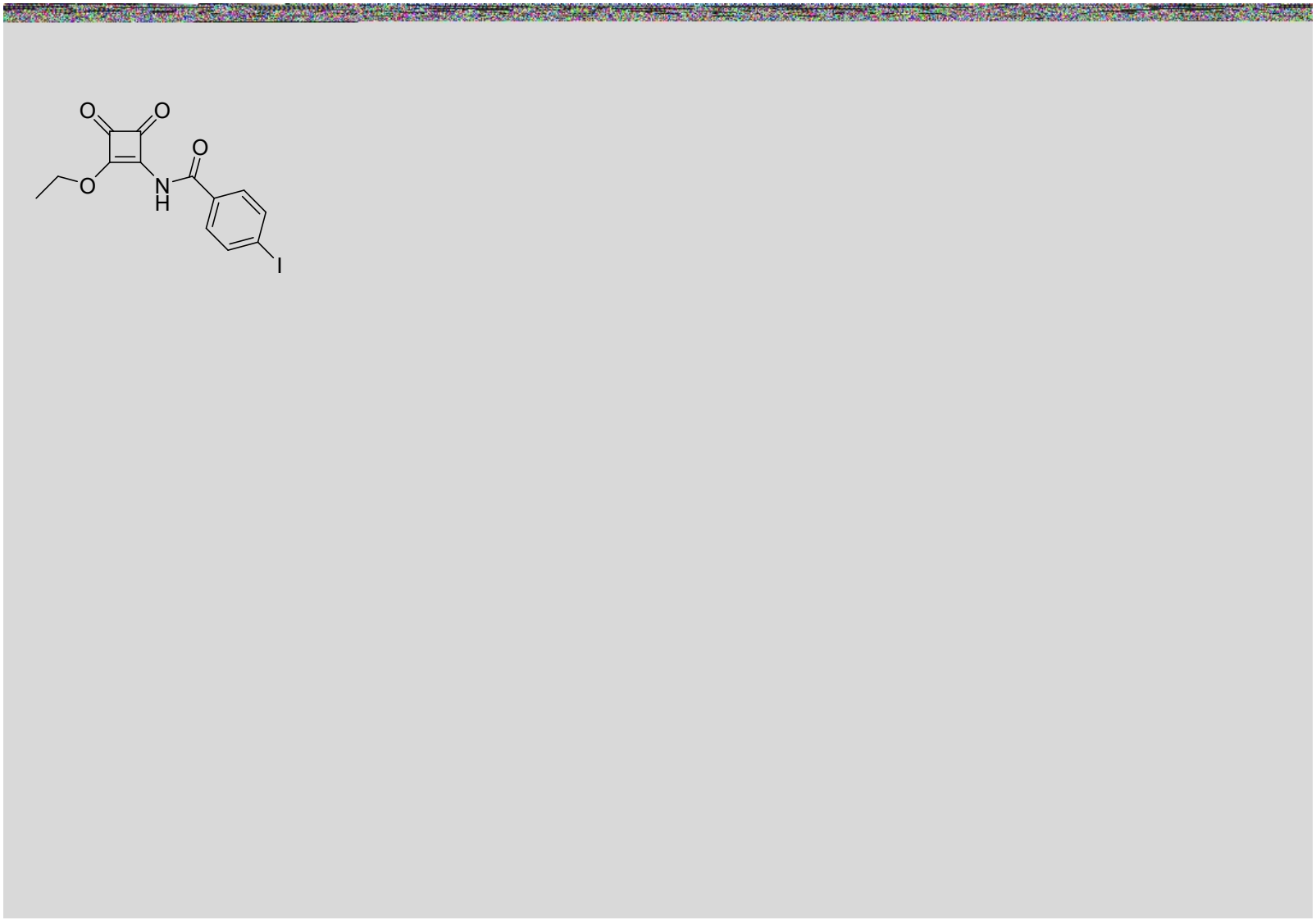


Figure S29. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***16****.*

Figure S30. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***16****.*

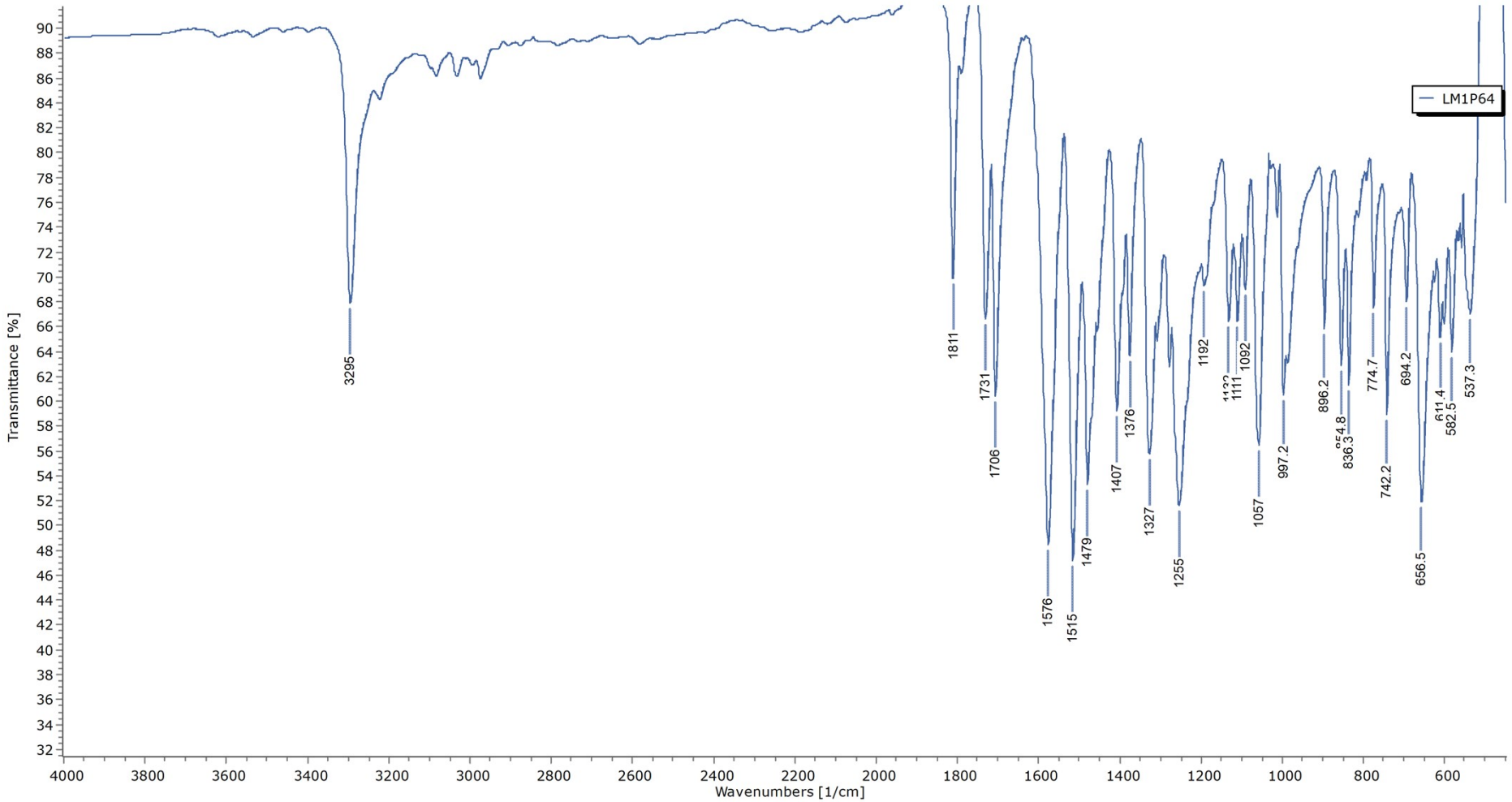
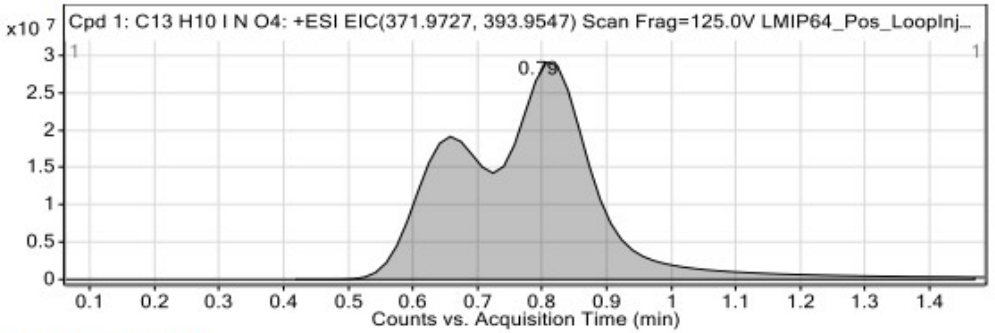


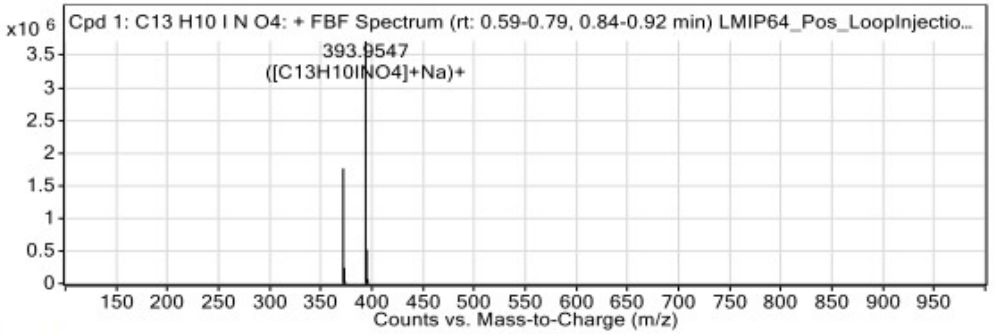
Figure S31. *IR spectrum of* ***16.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.42	0.79	1.47	27848282	399393219



Peak List

m/z	z	Abund	Formula	Ion
371.9727	1	1764381.38	C13H10INO4	(M+H)+
372.9758	1	242278.47	C13H10INO4	(M+H)+
373.9779	1	28882.52	C13H10INO4	(M+H)+
393.9547	1	3720356.25	C13H10INO4	(M+Na)+
394.9579	1	522127.16	C13H10INO4	(M+Na)+
395.96	1	66019.08	C13H10INO4	(M+Na)+
396.9621	1	5653.62	C13H10INO4	(M+Na)+

--- End Of Report ---

Figure S32. *HRMS of* ***16.***

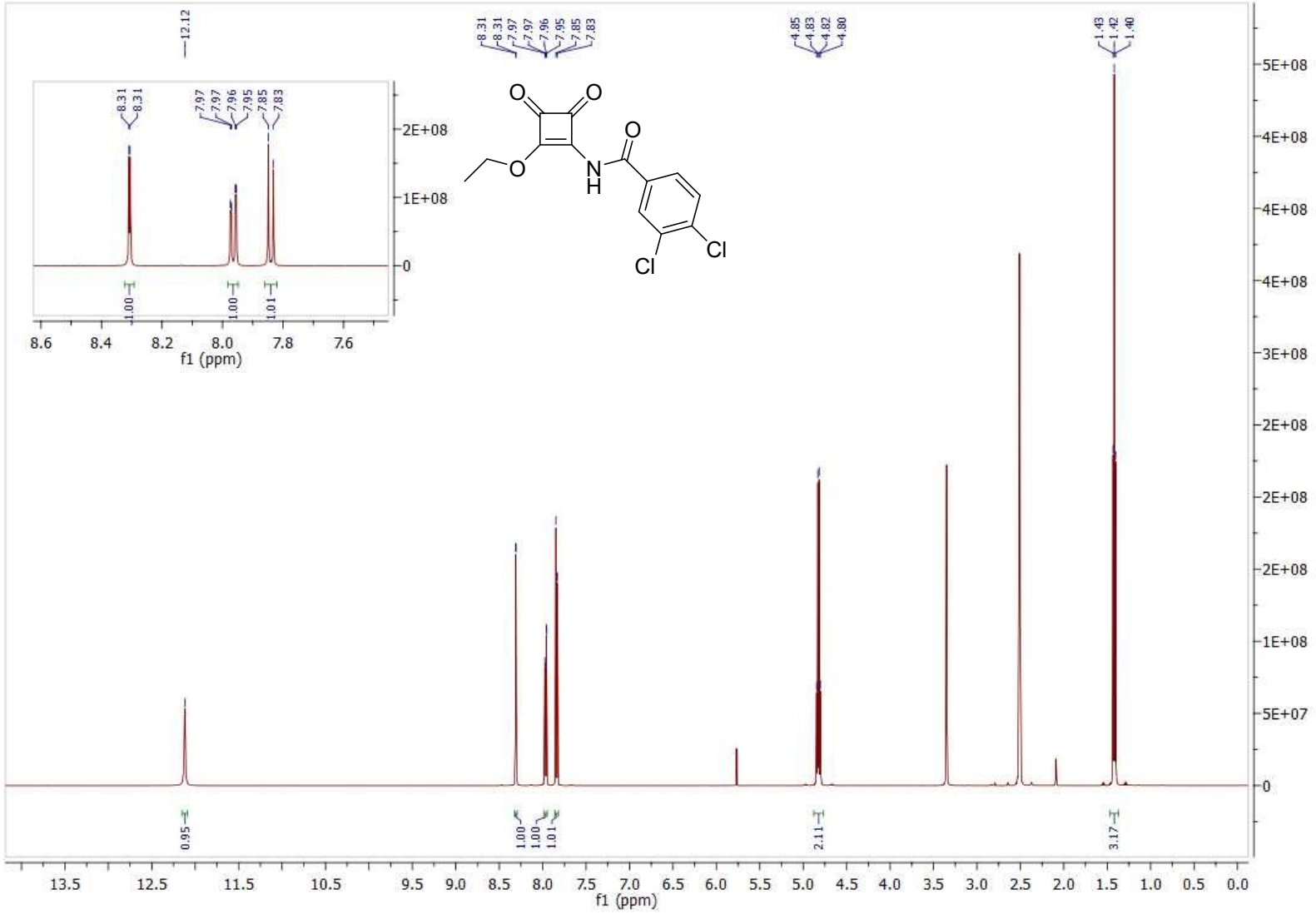


Figure S33. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***17****.*

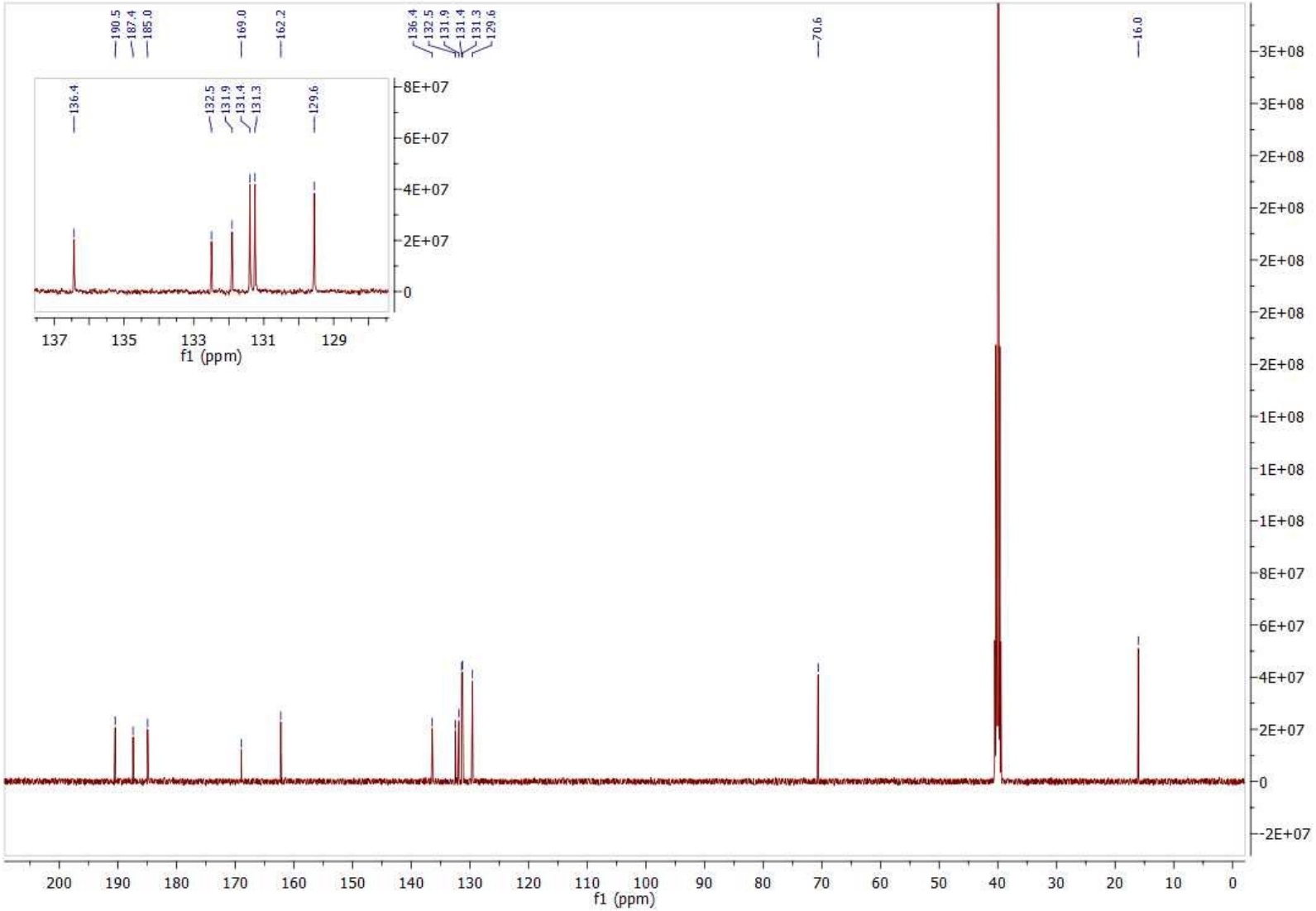


Figure S34. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***17****.*

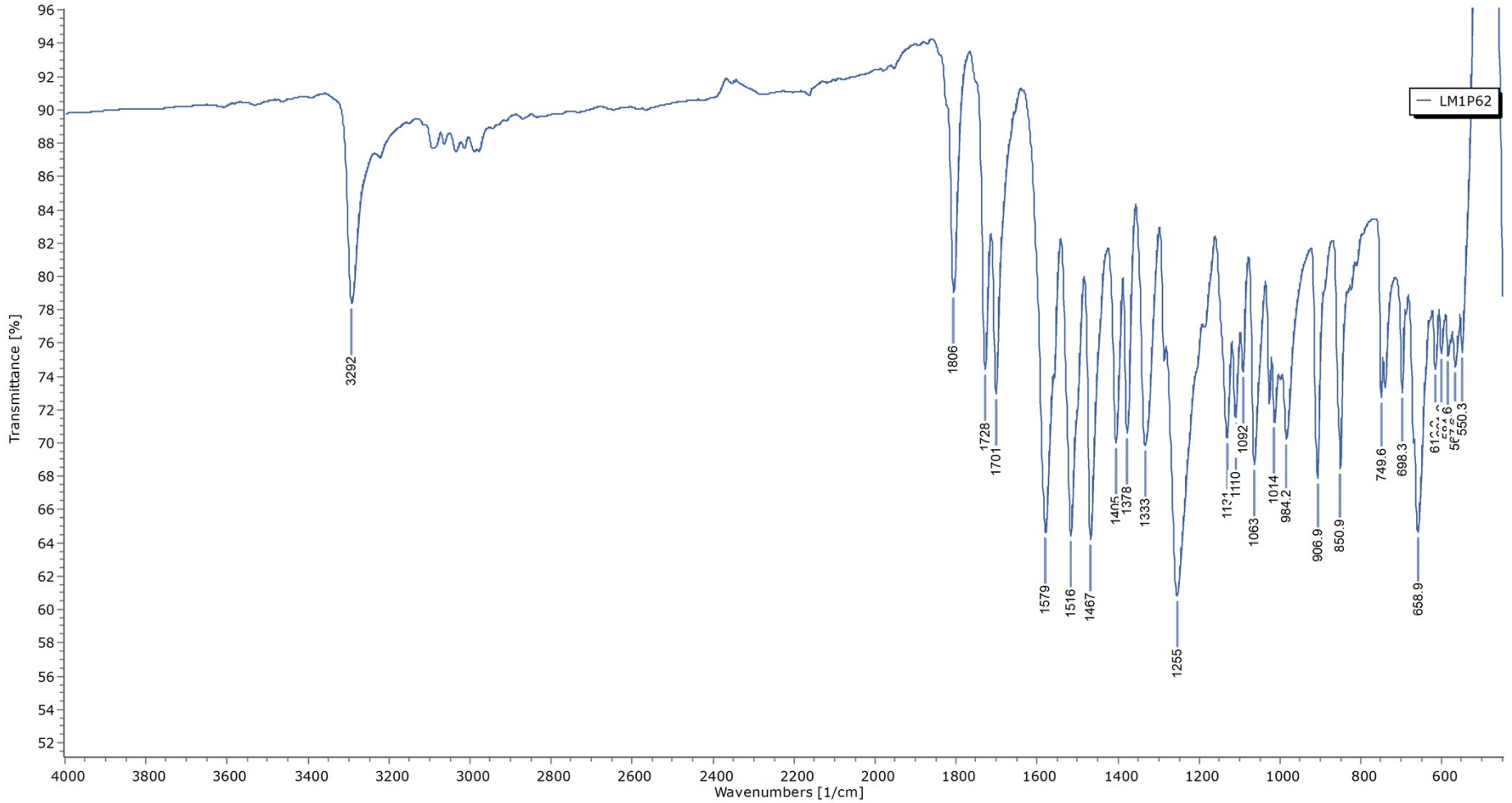
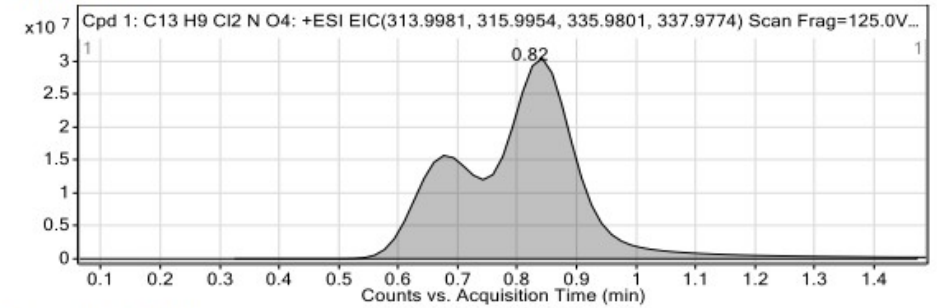


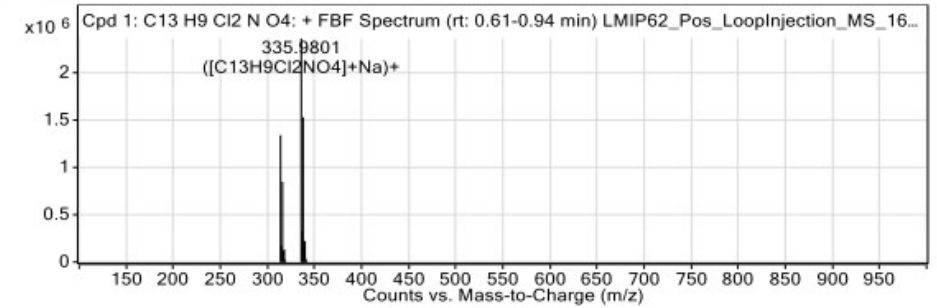
Figure S35. *IR spectrum of* ***17.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.32	0.82	1.47	26273803	367928171



Peak List

m/z	z	Abund	Formula	Ion
313.9982	1	1337021.75	C13H9Cl2NO4	(M+H)+
315.0014	1	176449.2	C13H9Cl2NO4	(M+H)+
315.9953	1	846996.31	C13H9Cl2NO4	(M+H)+
316.9993	1	116364.72	C13H9Cl2NO4	(M+H)+
317.9932	1	134404.78	C13H9Cl2NO4	(M+H)+
335.9801	1	2360401	C13H9Cl2NO4	(M+Na)+
336.9834	1	323599.44	C13H9Cl2NO4	(M+Na)+
337.9774	1	1525534.63	C13H9Cl2NO4	(M+Na)+
338.9806	1	194775.28	C13H9Cl2NO4	(M+Na)+
339.9752	1	222677.34	C13H9Cl2NO4	(M+Na)+

--- End Of Report ---

Figure S36. *HRMS of* ***17.***

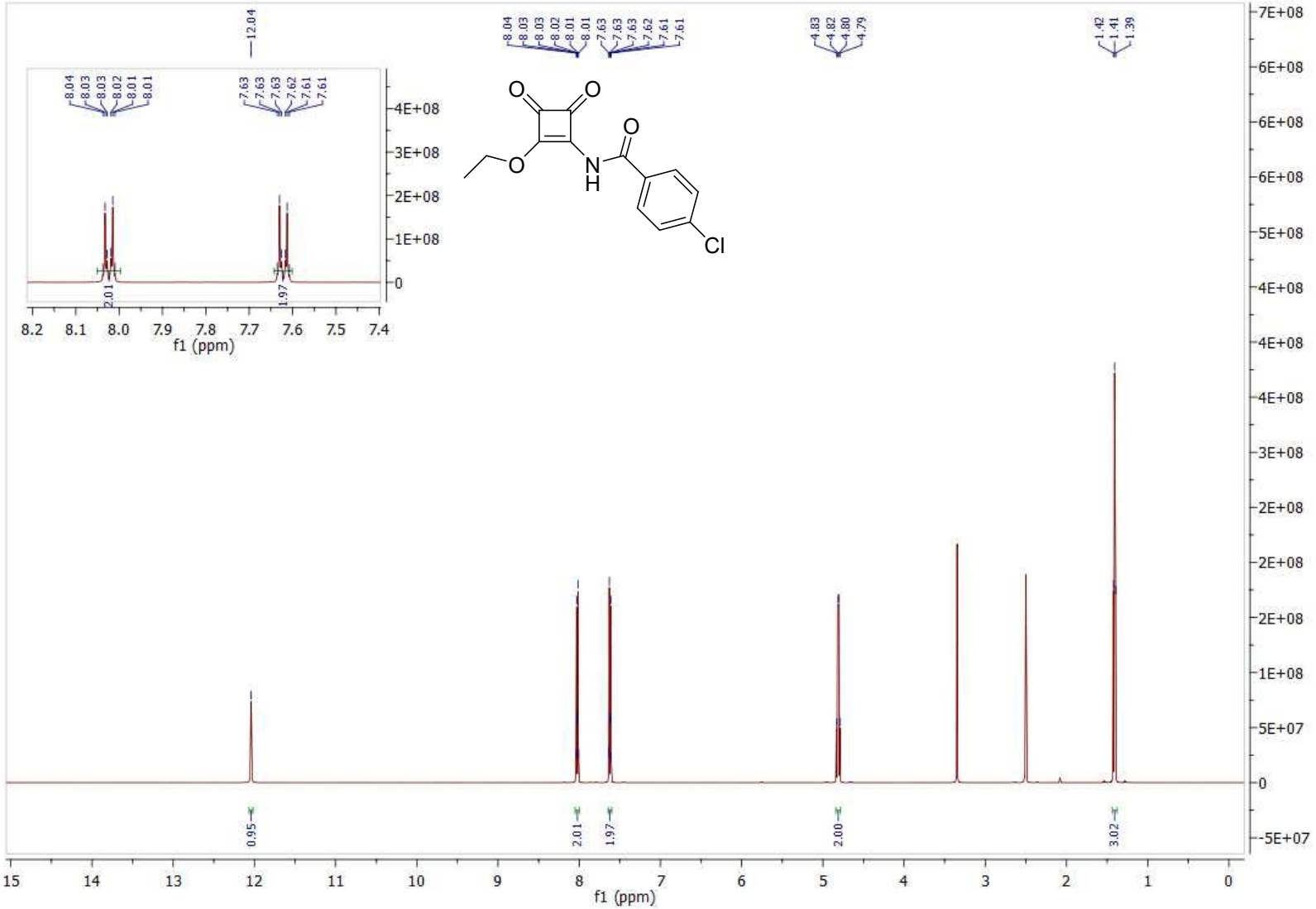


Figure S37. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***18.***

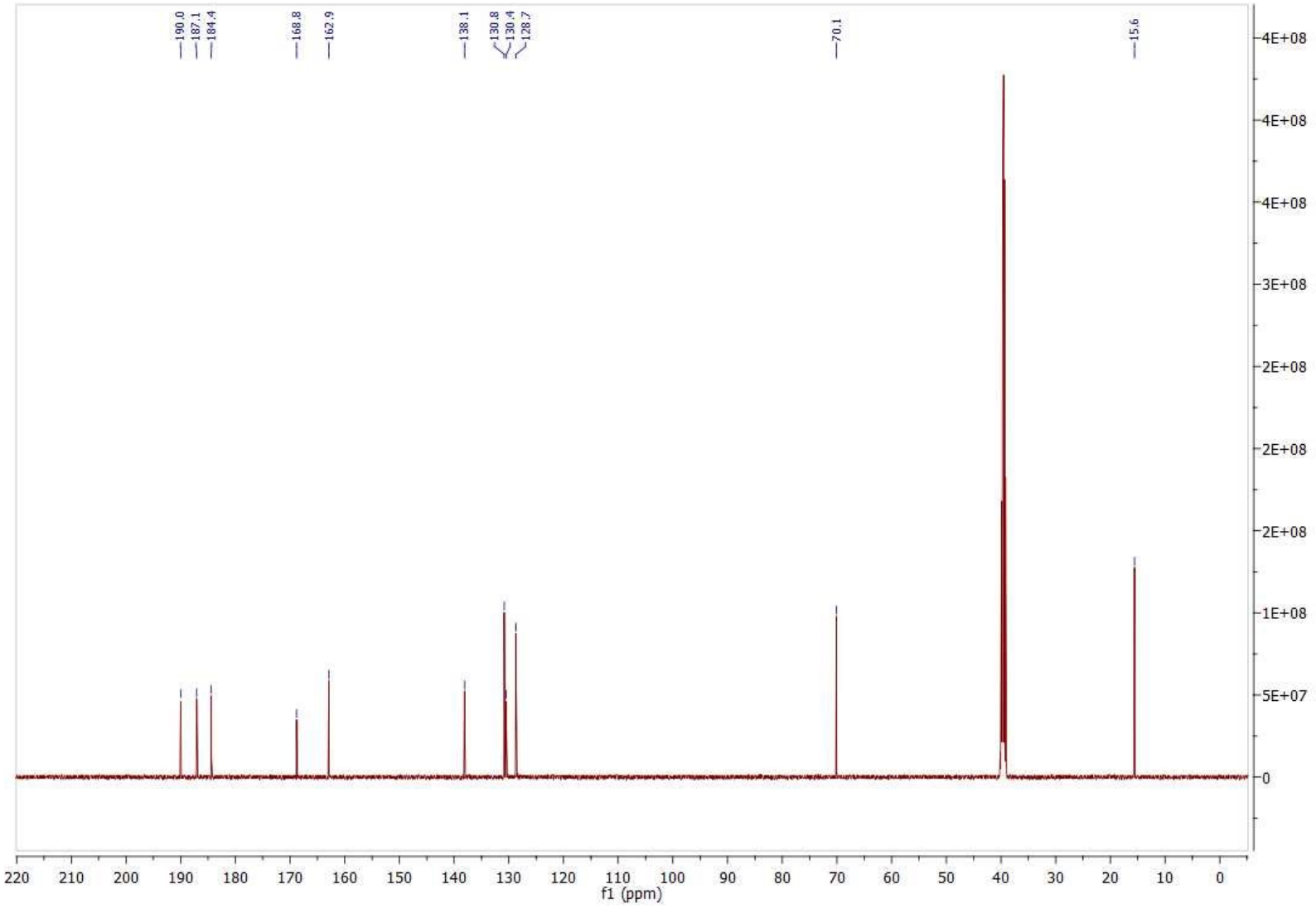


Figure S38. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of* ***18****.*

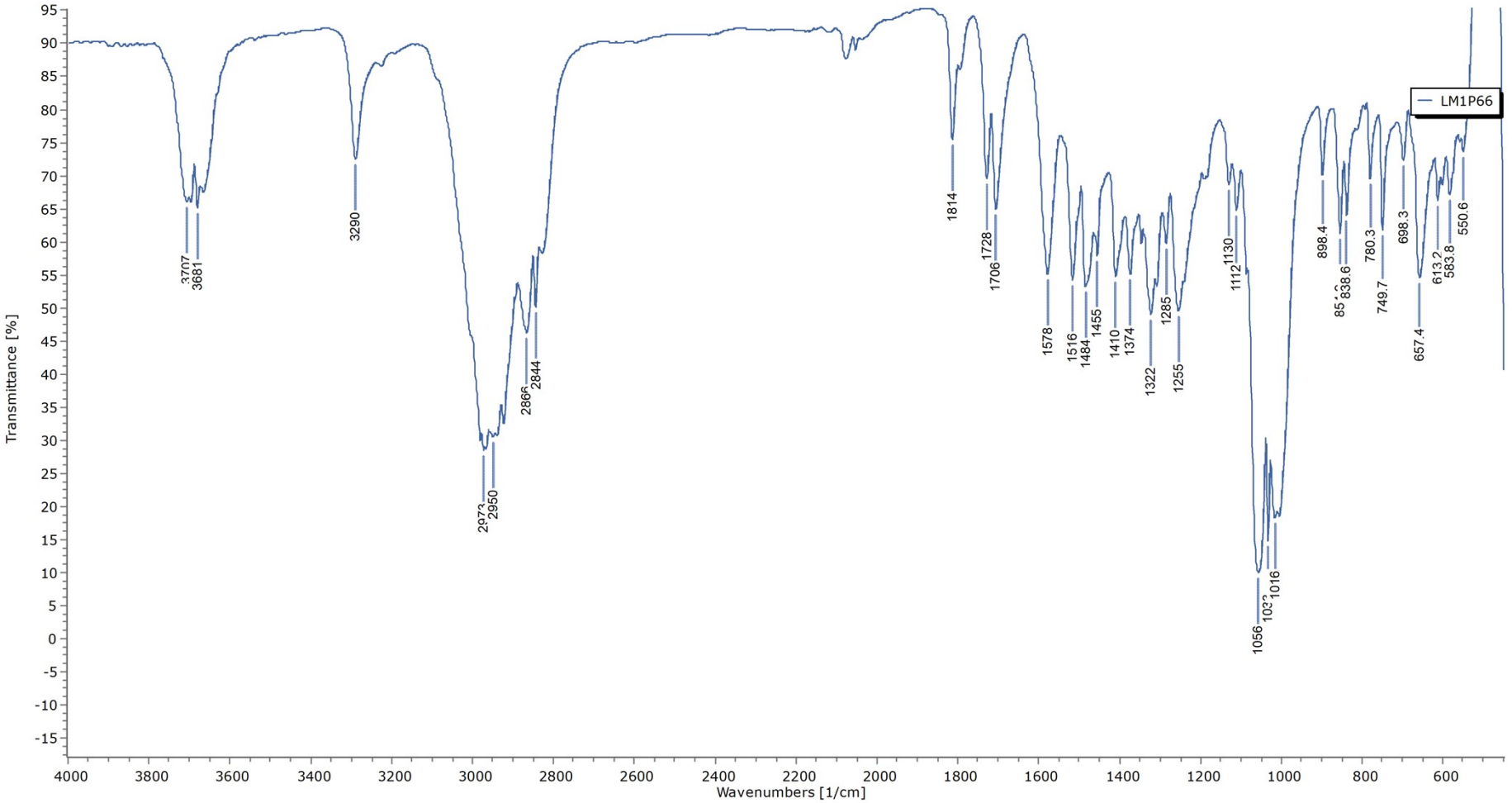
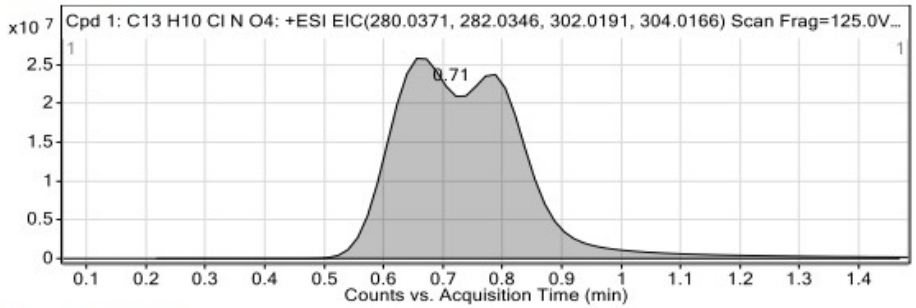


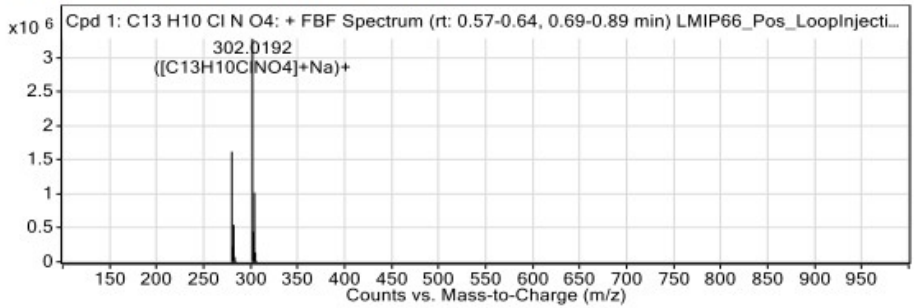
Figure S39. *IR spectrum of* ***18.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.22	0.71	1.47	25315312	386370120



Peak List

m/z	z	Abund	Formula	Ion
280.037	1	1620053	C13H10ClNO4	(M+H)+
281.0405	1	228181.17	C13H10ClNO4	(M+H)+
282.0346	1	543549.5	C13H10ClNO4	(M+H)+
283.0382	1	73518.92	C13H10ClNO4	(M+H)+
284.039	1	10691.38	C13H10ClNO4	(M+H)+
302.0192	1	3282117.5	C13H10ClNO4	(M+Na)+
303.0224	1	444767.75	C13H10ClNO4	(M+Na)+
304.0164	1	1017450.31	C13H10ClNO4	(M+Na)+
305.0197	1	139950.11	C13H10ClNO4	(M+Na)+
306.0213	1	17136.4	C13H10ClNO4	(M+Na)+

--- End Of Report ---

Figure S40. *HRMS of* ***18.***

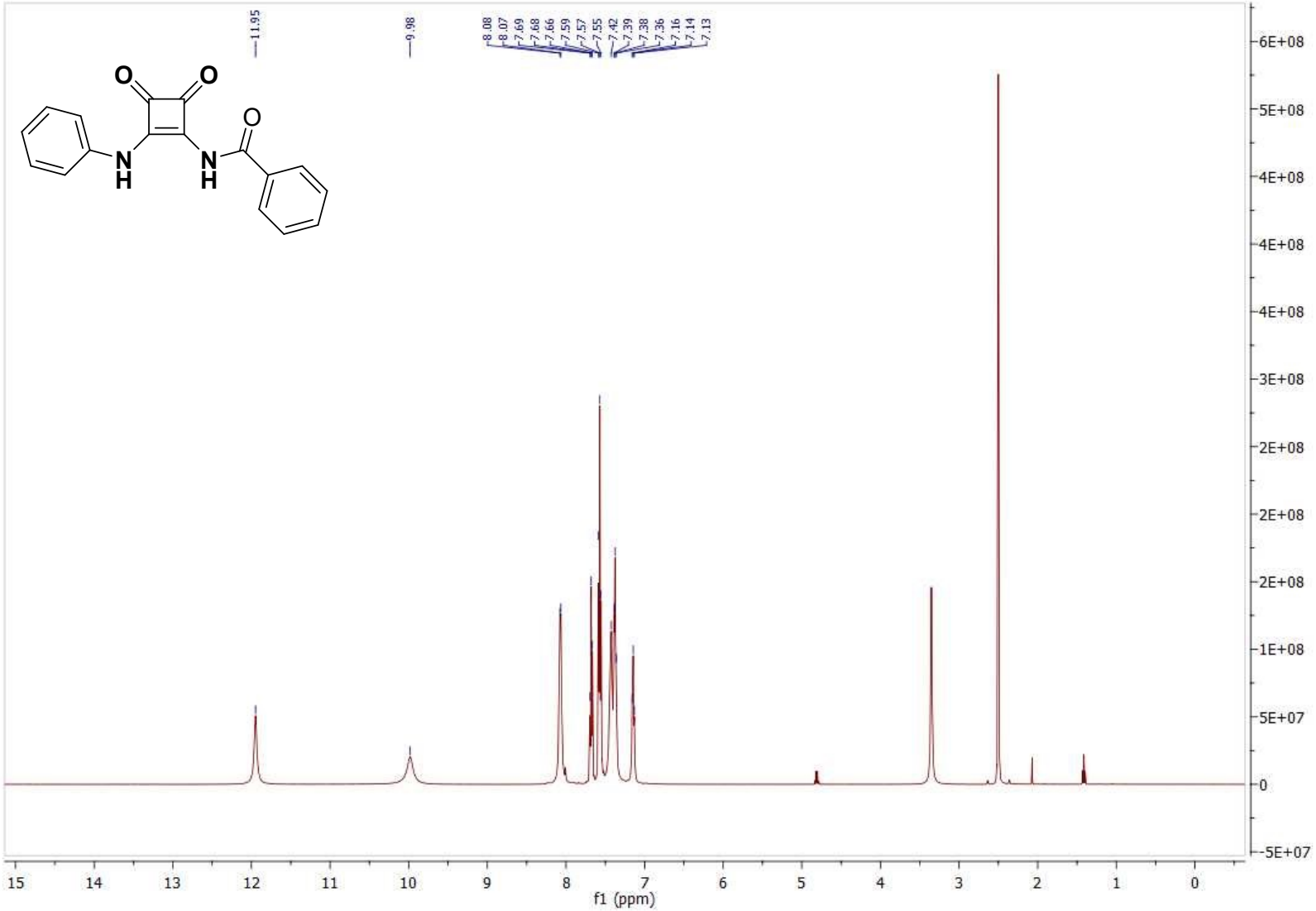


Figure S41. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***1****.*

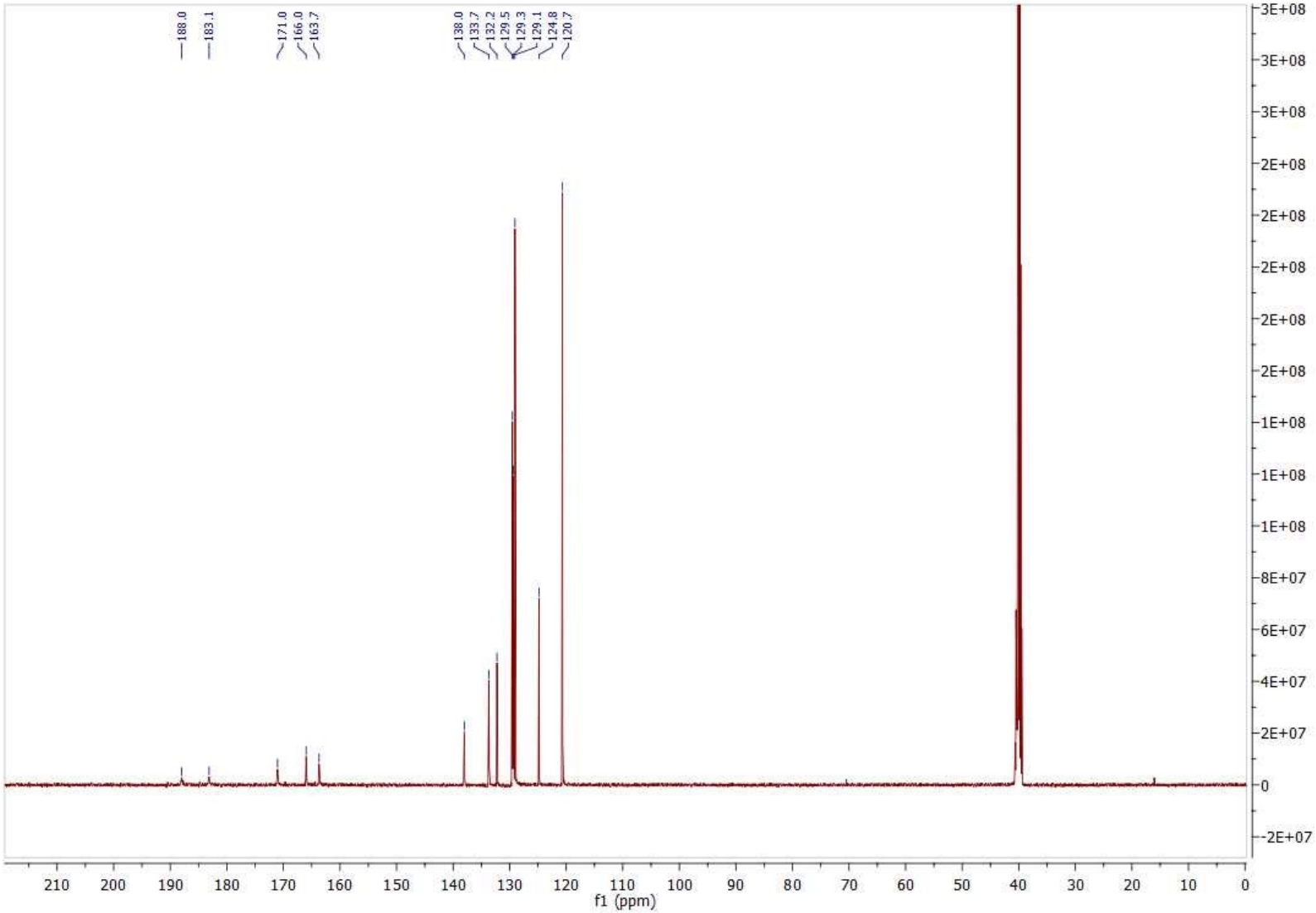


Figure S42. ^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of **1**.

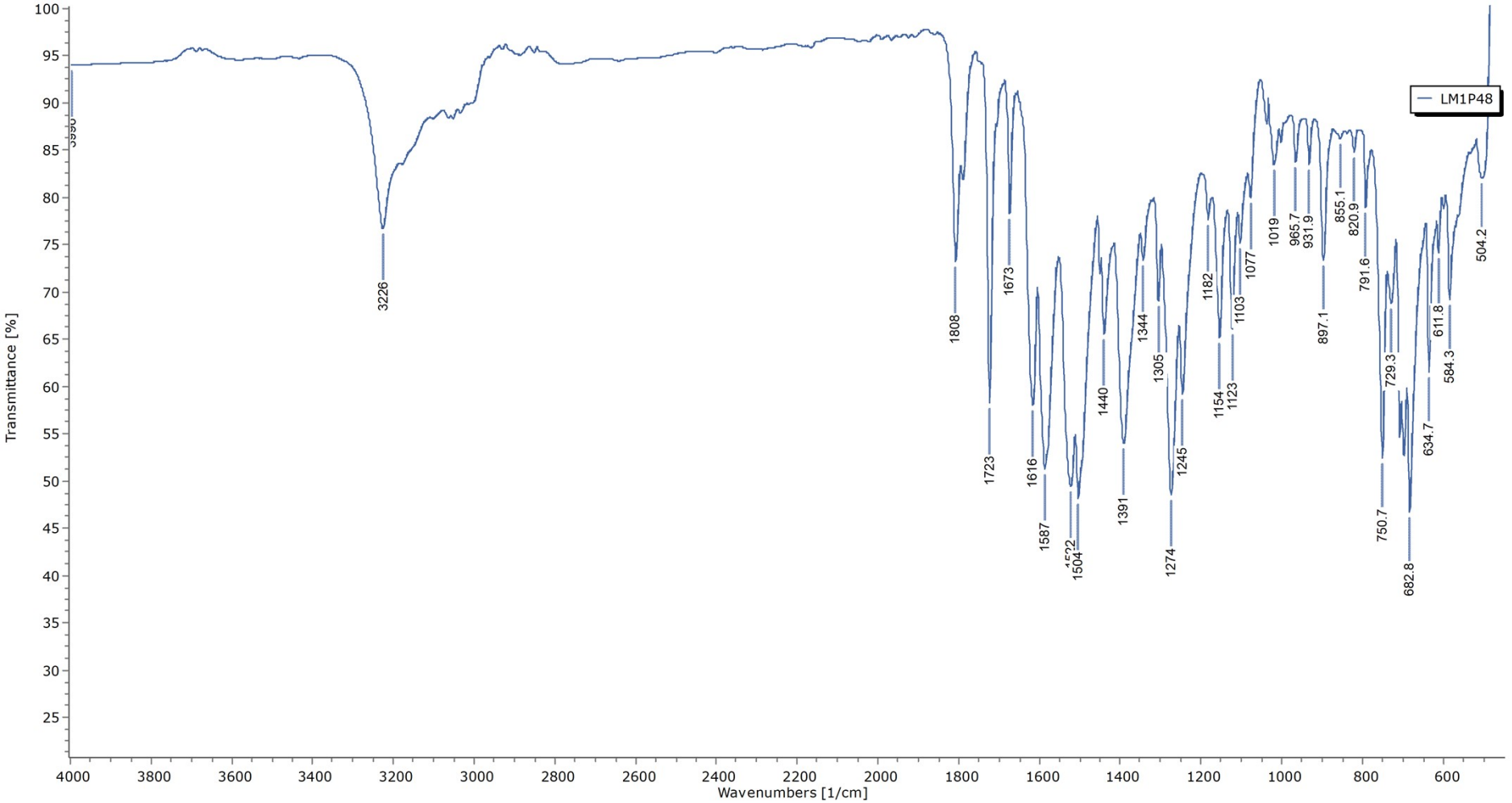
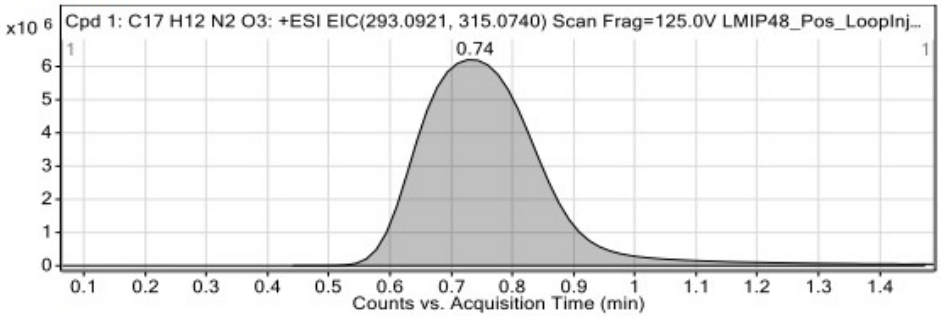


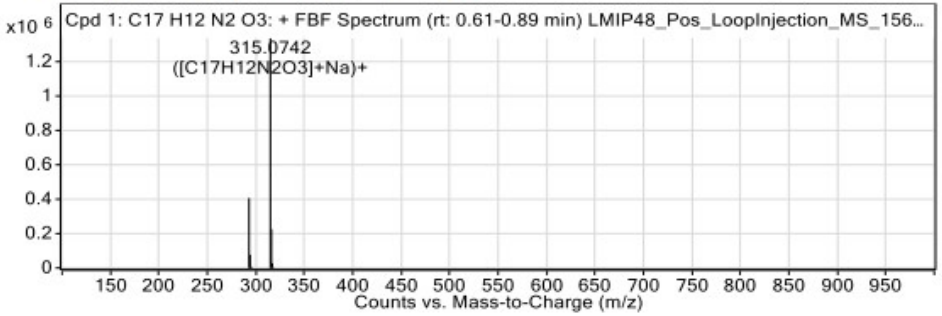
Figure S43. *IR spectrum of* ***1.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.44	0.74	1.47	6065743	84953217



Peak List

m/z	z	Abund	Formula	Ion
293.0926	1	407026.53	C17H12N2O3	(M+H)+
294.0955	1	76758.41	C17H12N2O3	(M+H)+
295.0992	1	9511.4	C17H12N2O3	(M+H)+
296.1039	1	895.61	C17H12N2O3	(M+H)+
315.0742	1	1339016.38	C17H12N2O3	(M+Na)+
316.0776	1	226085.53	C17H12N2O3	(M+Na)+
317.0805	1	27438.29	C17H12N2O3	(M+Na)+
318.0829	1	2875.02	C17H12N2O3	(M+Na)+

--- End Of Report ---

Figure S44. HRMS of **1.**

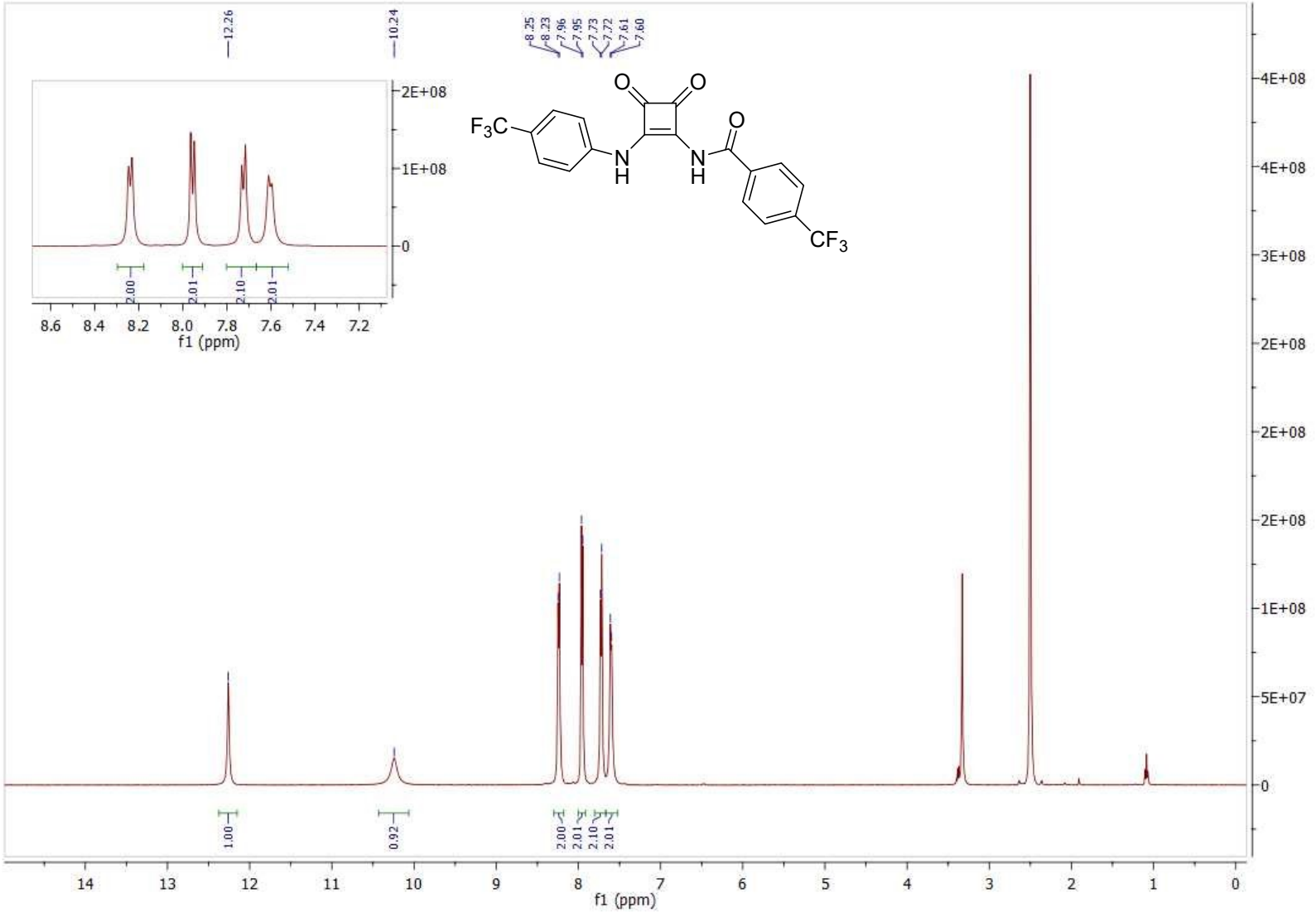


Figure S45. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***2****.*

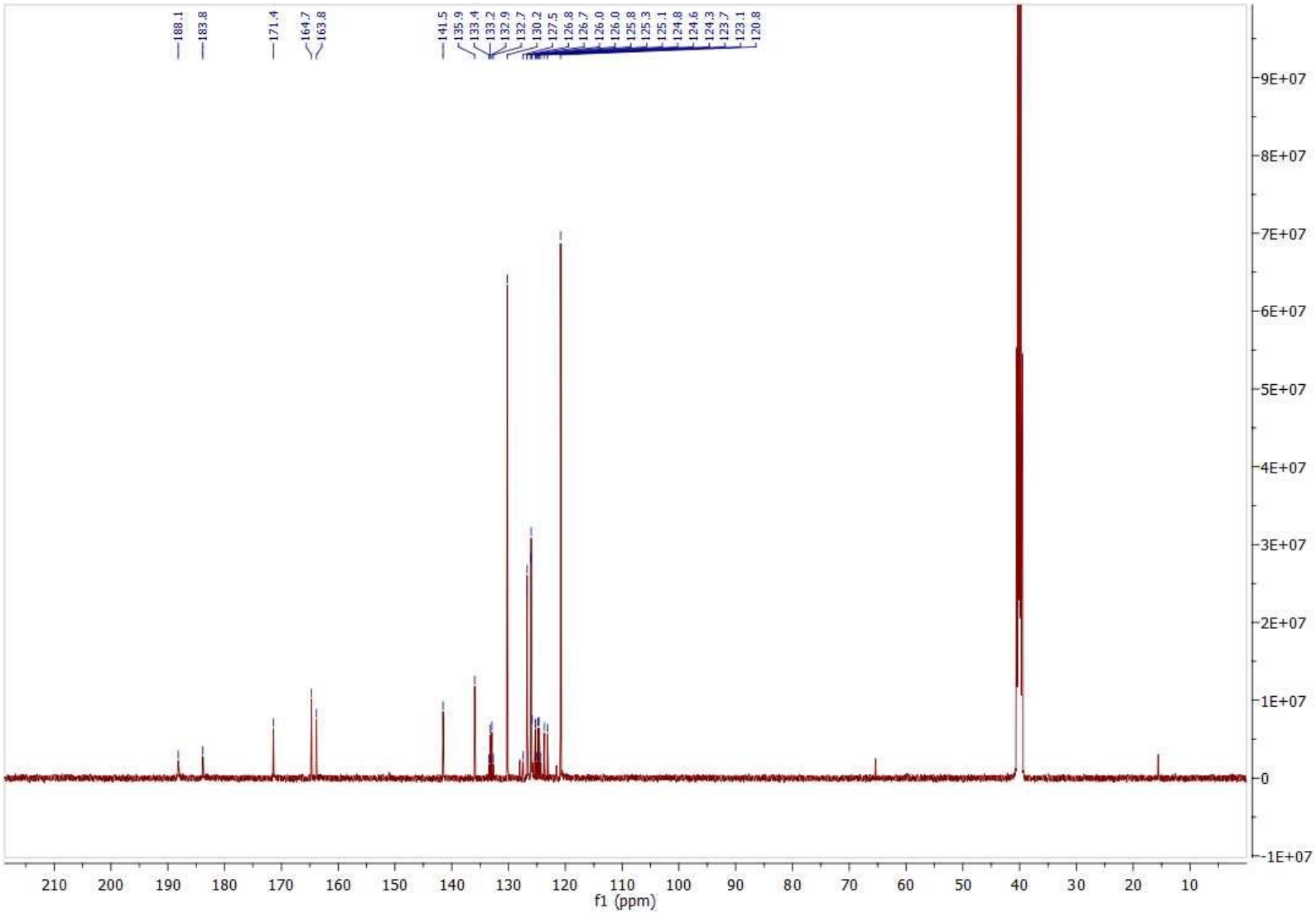


Figure S46. ^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of **2**.

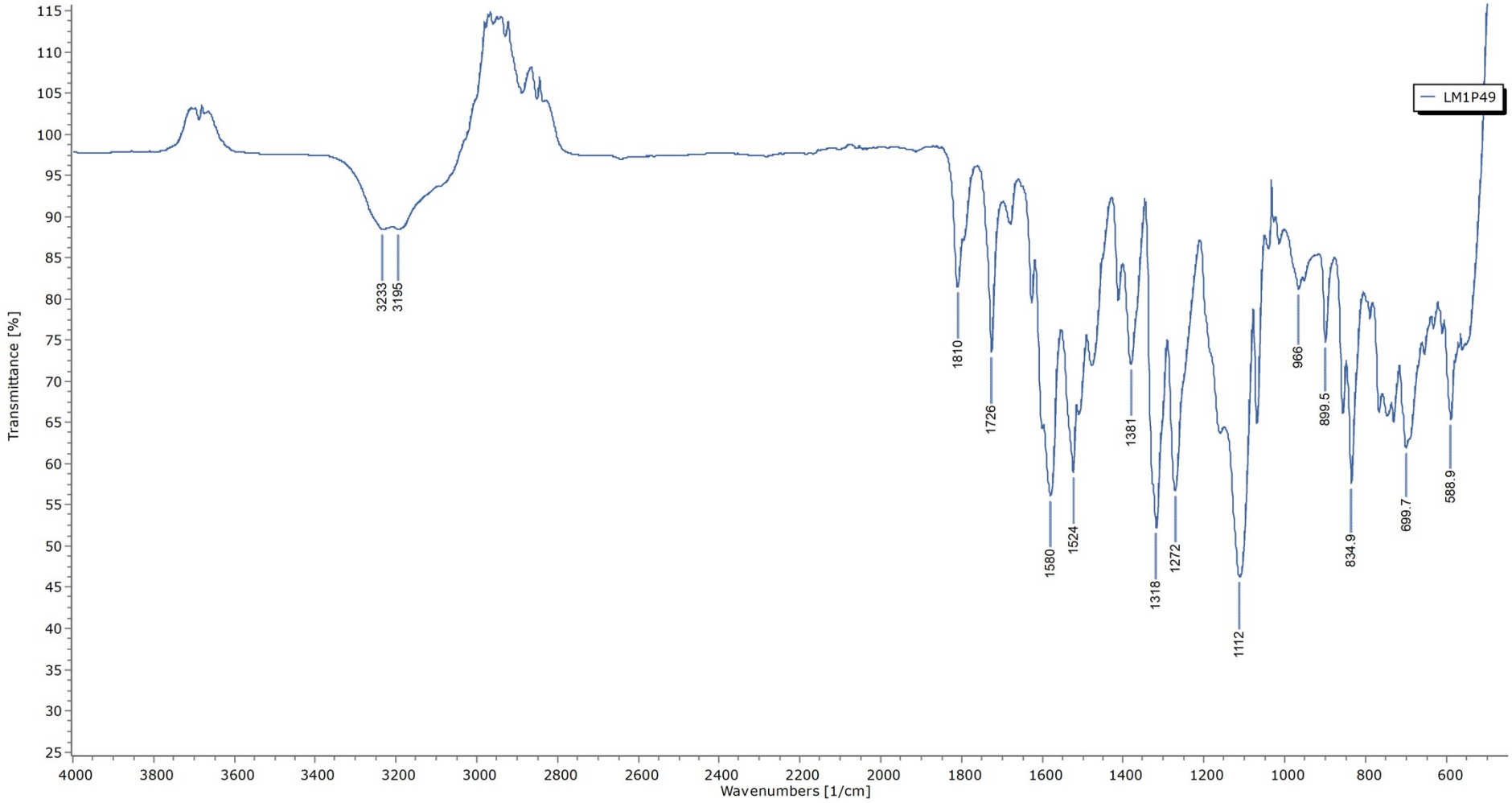
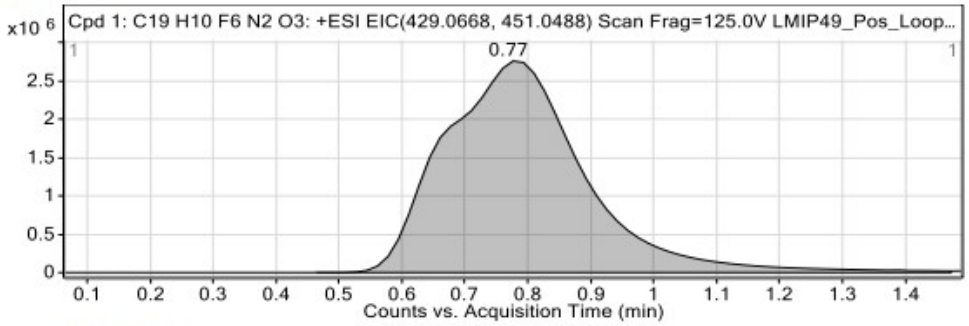


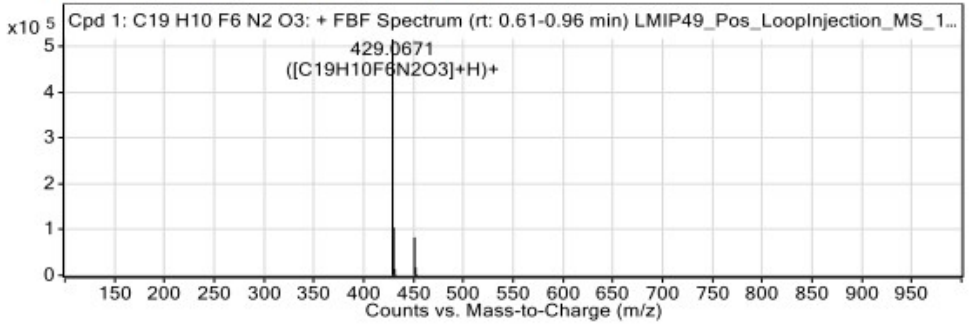
Figure S47. IR spectrum of **2.**

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.46	0.77	1.47	2565745	42556804



Peak List

m/z	z	Abund	Formula	Ion
429.0671	1	516063.66	C19H10F6N2O3	(M+H)+
430.0702	1	104402.95	C19H10F6N2O3	(M+H)+
431.0725	1	14208.69	C19H10F6N2O3	(M+H)+
432.0748	1	1429.52	C19H10F6N2O3	(M+H)+
451.0488	1	82831.23	C19H10F6N2O3	(M+Na)+
452.0518	1	17284.08	C19H10F6N2O3	(M+Na)+
453.0548	1	2438.04	C19H10F6N2O3	(M+Na)+
454.0573	1	228.05	C19H10F6N2O3	(M+Na)+

--- End Of Report ---

Figure S48. HRMS of **2**

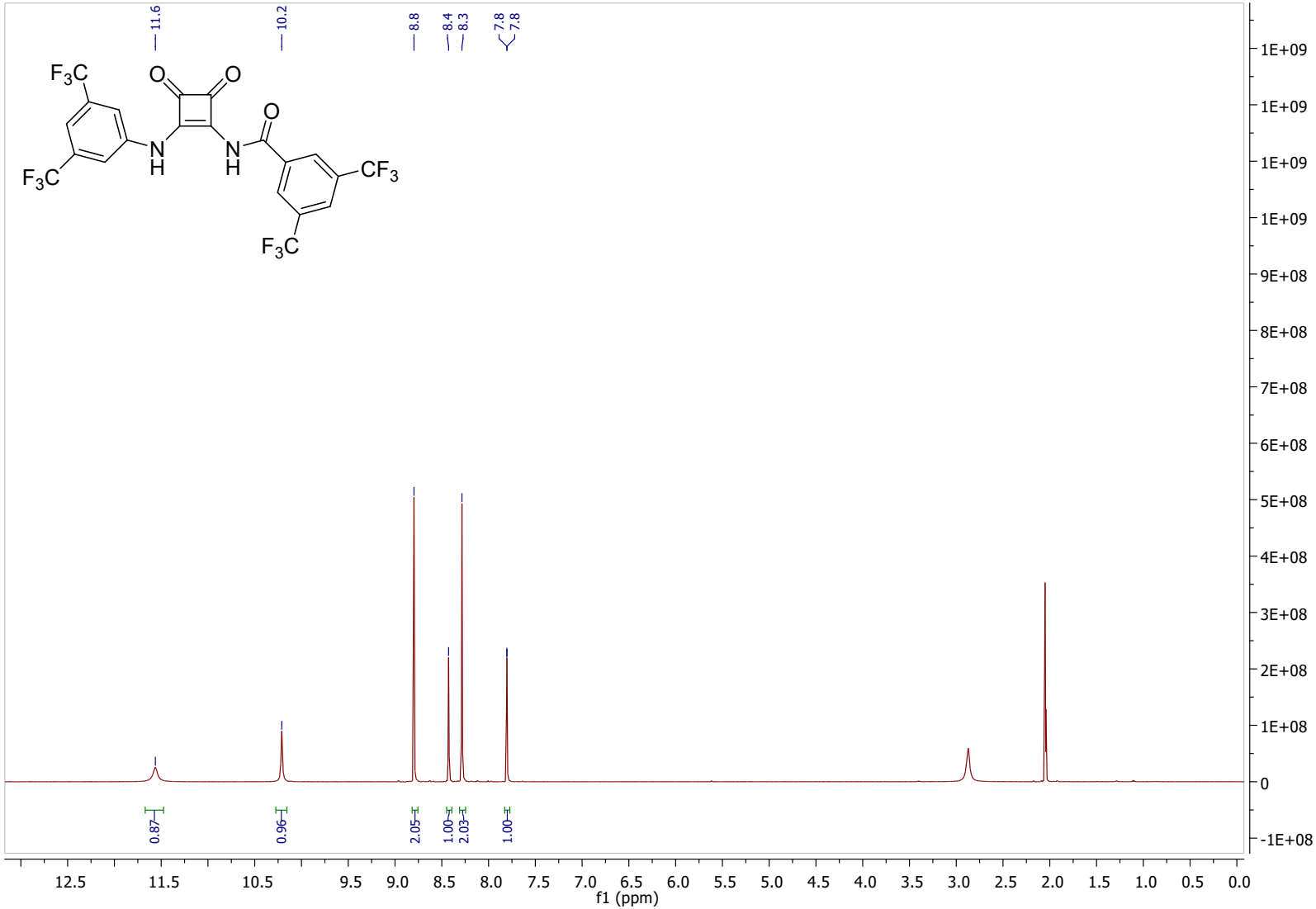


Figure S49. *^{1}H NMR ($(CD_3)_2CO$-d_6, 500 MHz) spectrum of* ***3****.*

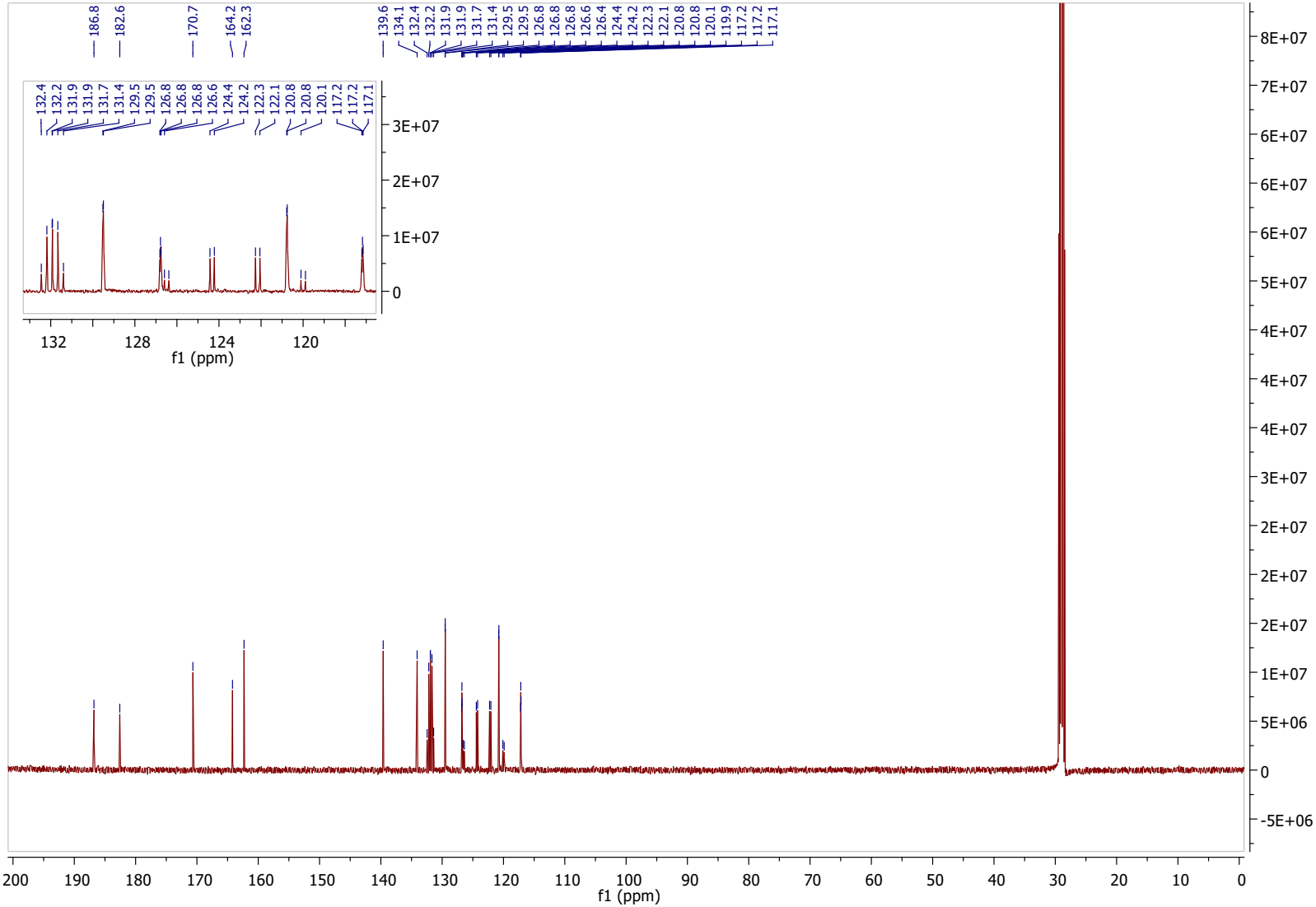


Figure S50. ^{13}C NMR ($(CD_3)_2CO$-d_6, 126 MHz) spectrum of **3**.

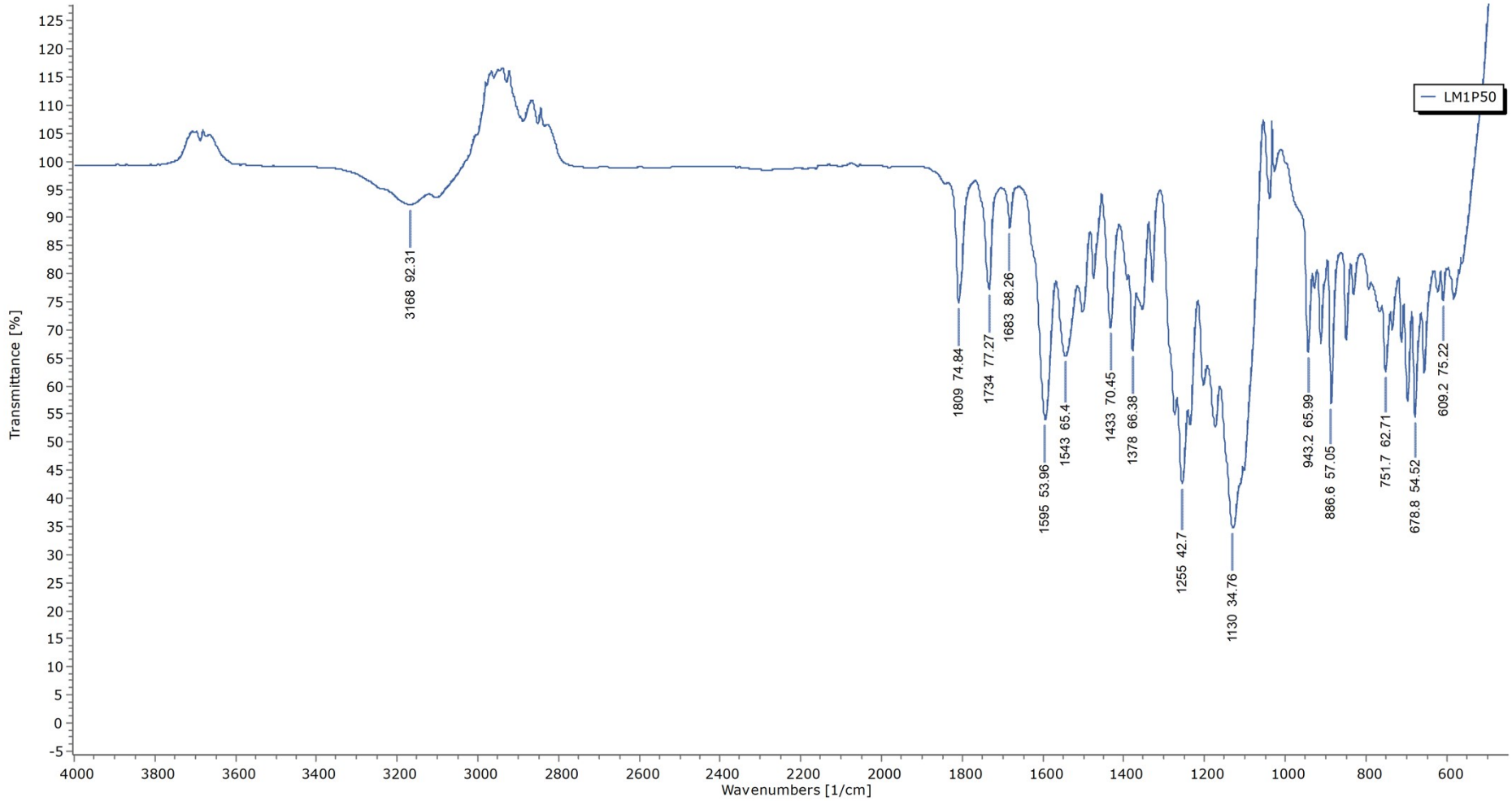
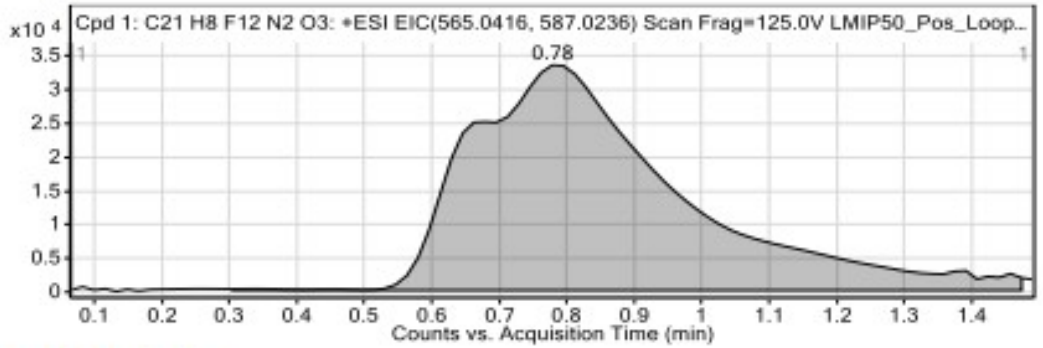


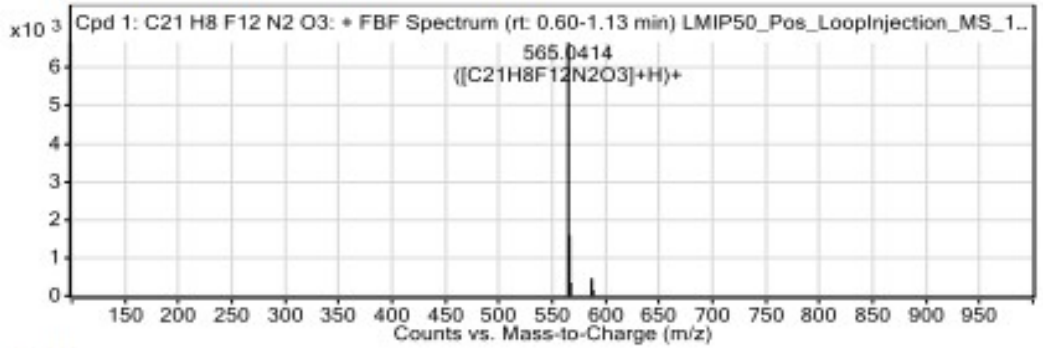
Figure S51. IR spectrum of **3.**

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.3	0.78	1.47	31268	718740



Peak List

m/z	z	Abund	Formula	Ion
565.0414	1	6662.23	C21H8F12N2O3	(M+H)+
566.0449	1	1596.42	C21H8F12N2O3	(M+H)+
567.0472	1	348.42	C21H8F12N2O3	(M+H)+
587.023	1	464.75	C21H8F12N2O3	(M+Na)+
588.0256	1	152.73	C21H8F12N2O3	(M+Na)+

--- End Of Report ---

Figure S52. HRMS of **3.**

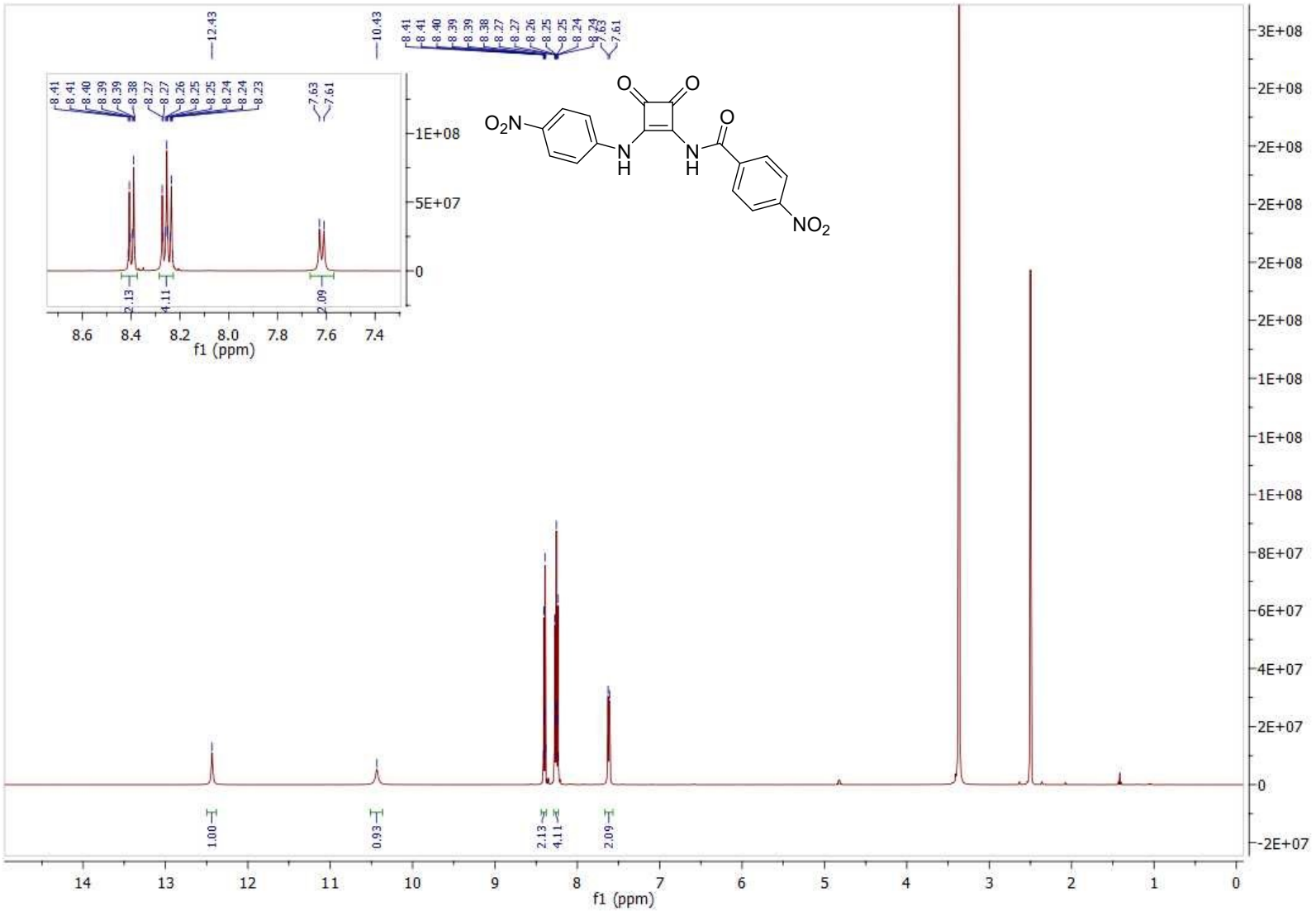


Figure S53. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***4****.*

Figure S54. ^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of **4**.

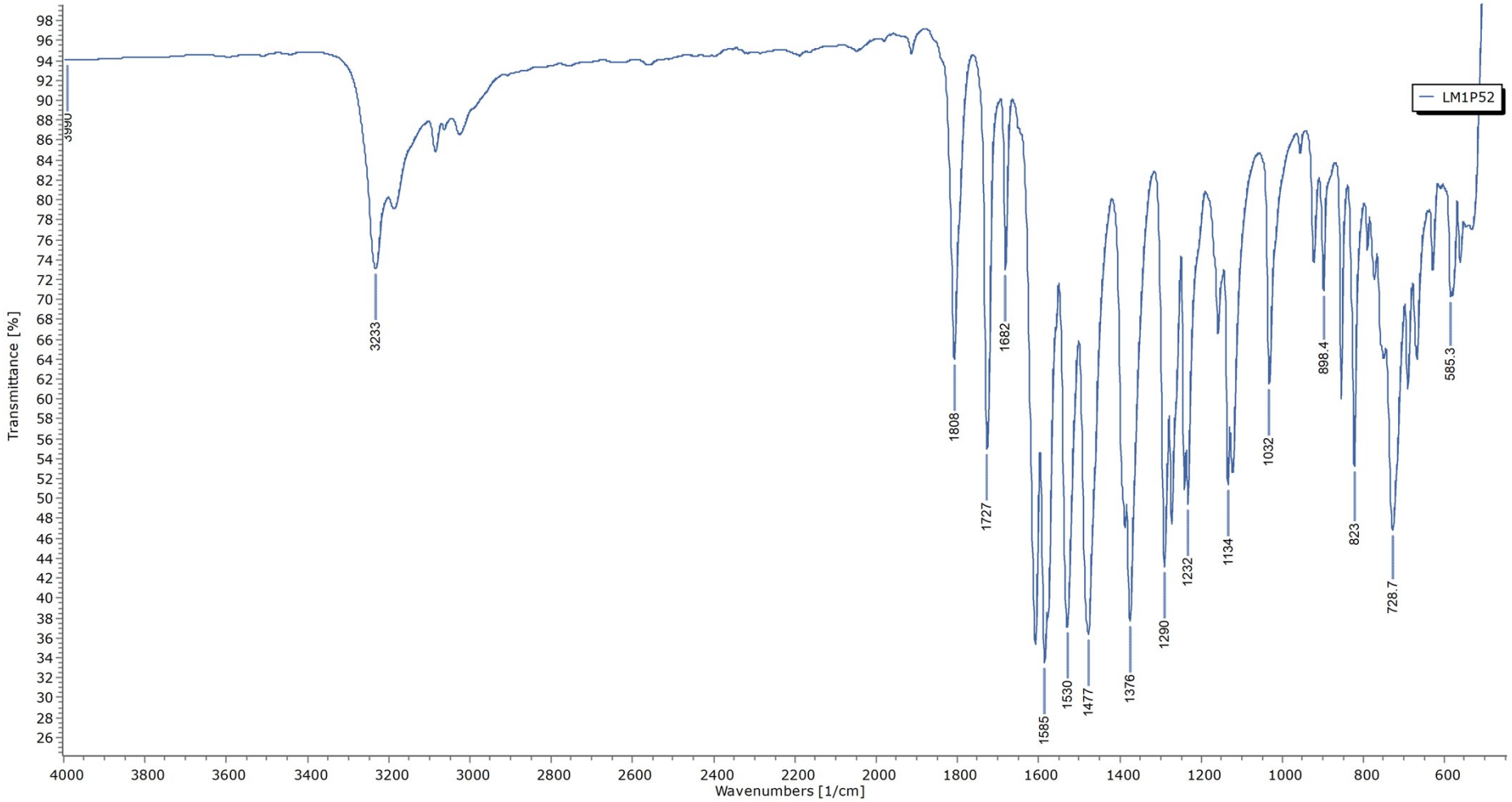
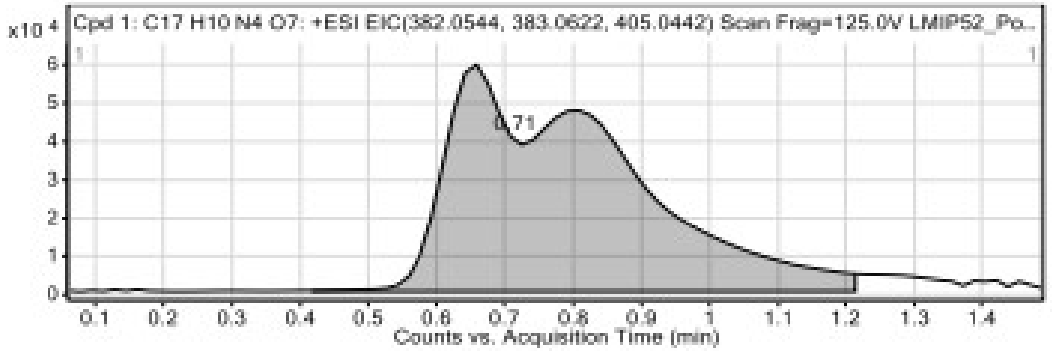
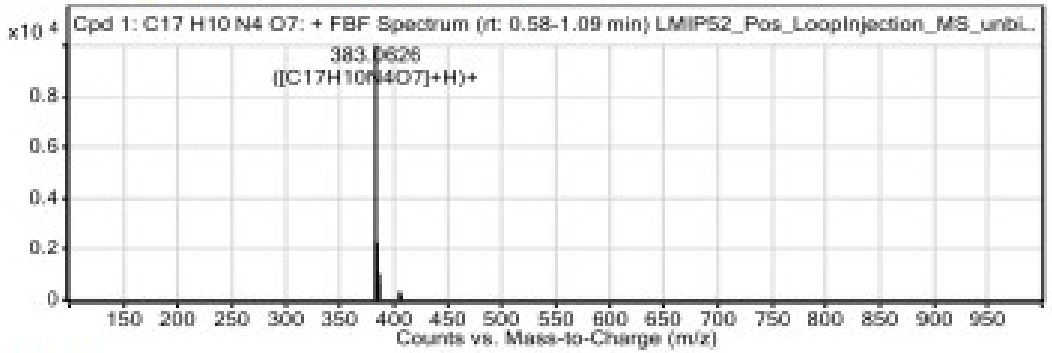


Figure S55. IR spectrum of **4.**



Integration Peak List

Start	RT	End	Height	Area
0.42	0.71	1.21	51518	1056805



Peak List

m/z	z	Abund	Formula	Ion
383.0626	1	10051.52	C17H10N4O7	(M+H)+
384.0661	1	2283.79	C17H10N4O7	(M+H)+
385.0708	1	617.55	C17H10N4O7	(M+H)+
386.0813	1	1026.47	C17H10N4O7	(M+H)+
405.0449	1	334.57	C17H10N4O7	(M+Na)+
406.0365	1	213.53	C17H10N4O7	(M+Na)+

--- End Of Report ---

Figure S56. HRMS of **4.**

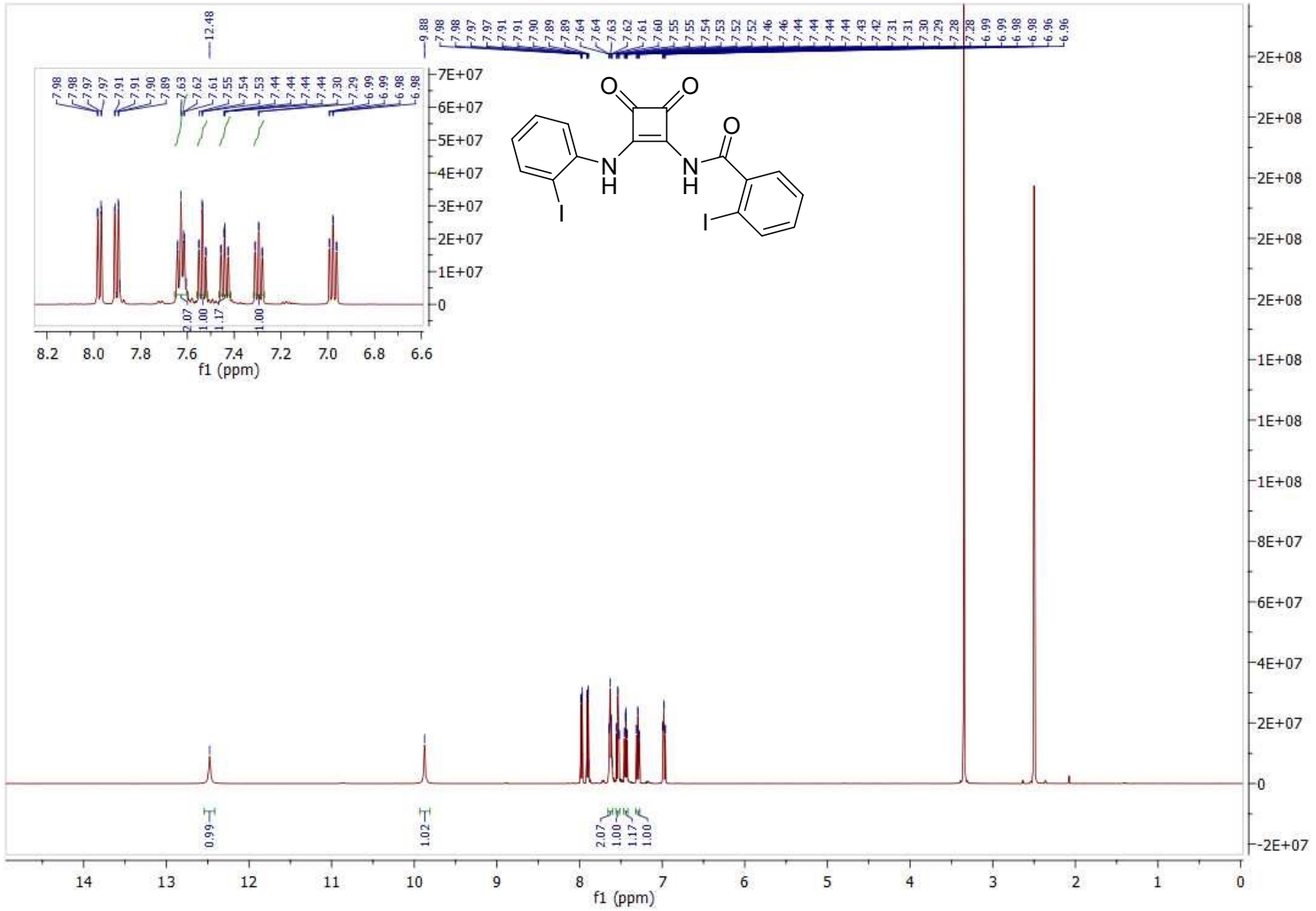


Figure S57. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***5****.*

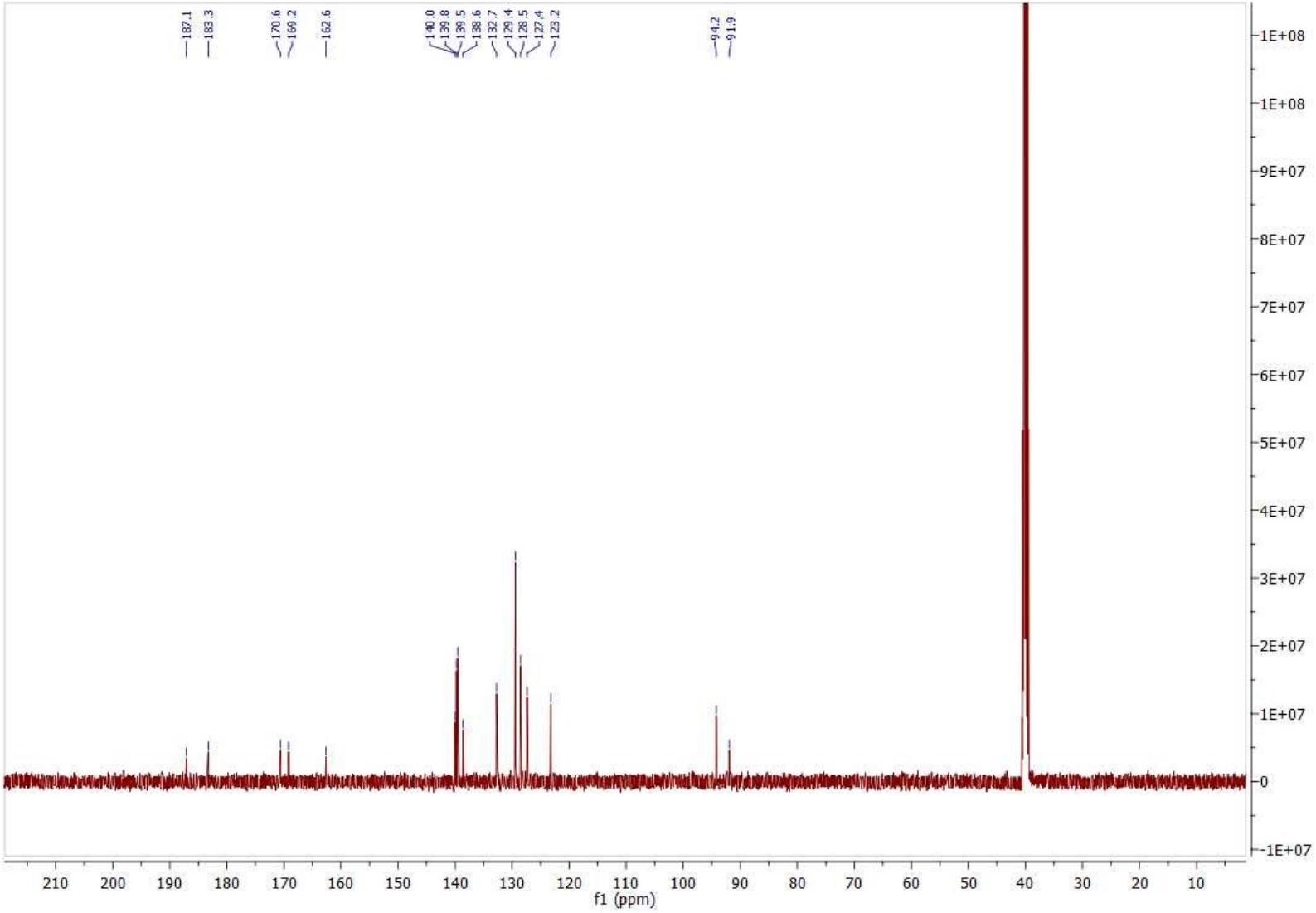


Figure 58. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of **5**.*

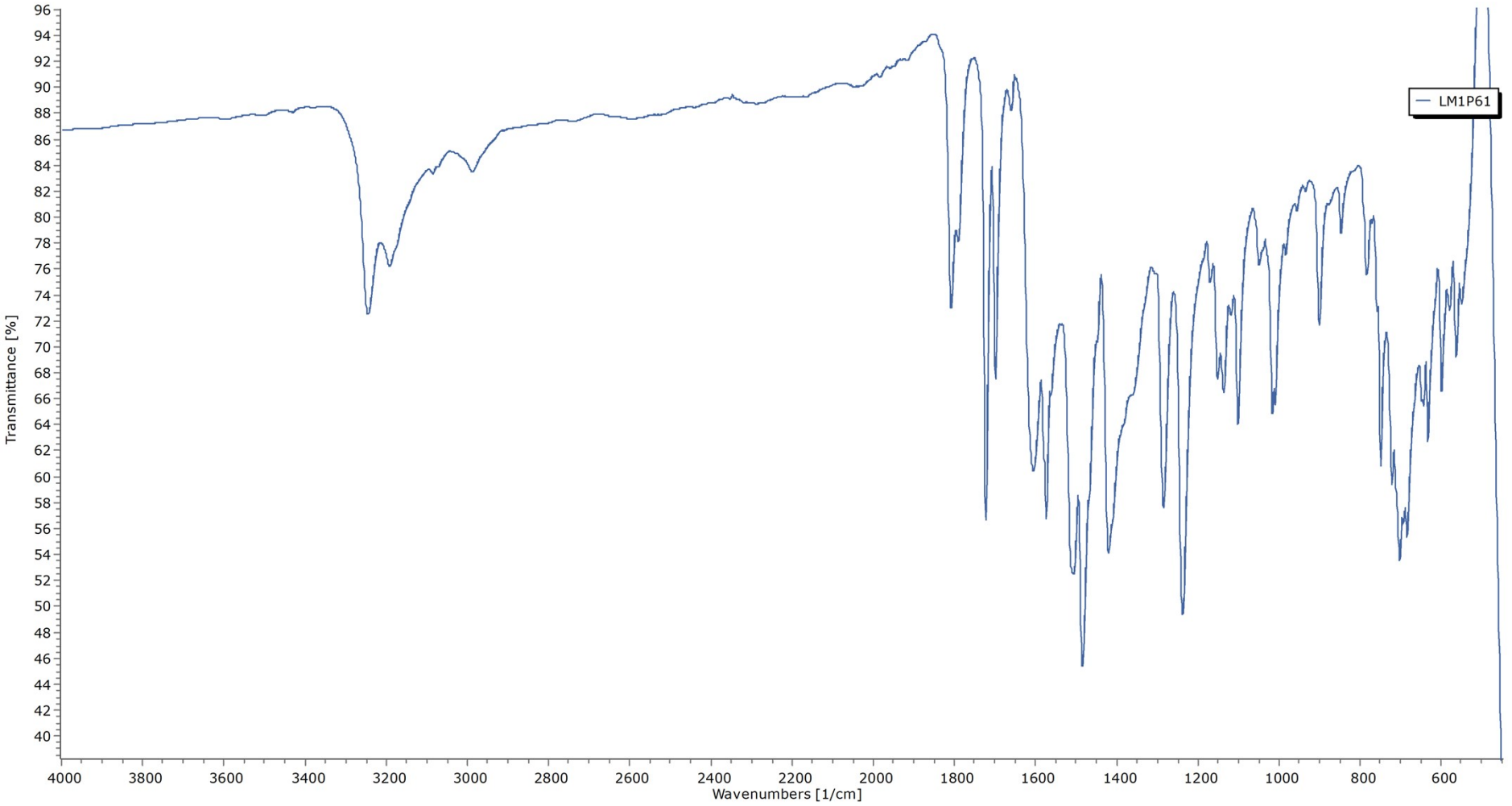
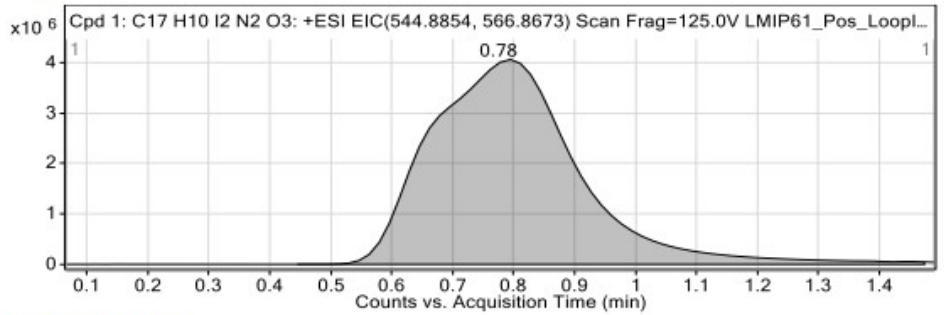


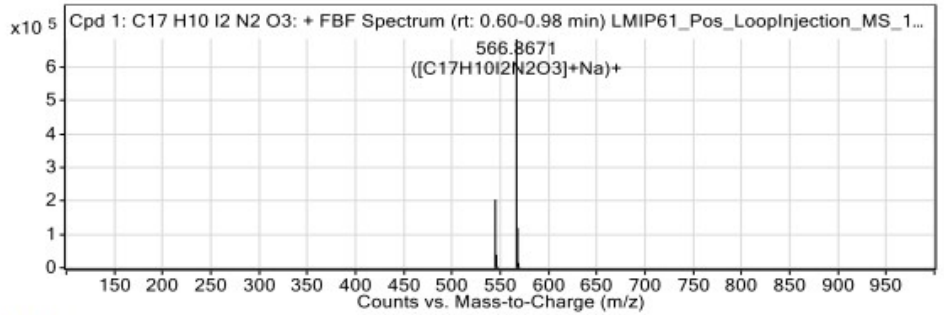
Figure S59. *IR spectrum of* ***5.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.45	0.78	1.47	3793140	68013276



Peak List

m/z	z	Abund	Formula	Ion
544.8851	1	204029.7	C17H10I2N2O3	(M+H)+
545.888	1	39219.65	C17H10I2N2O3	(M+H)+
546.8907	1	4593.09	C17H10I2N2O3	(M+H)+
547.8918	1	444.34	C17H10I2N2O3	(M+H)+
566.8671	1	684266.06	C17H10I2N2O3	(M+Na)+
567.8701	1	118774.71	C17H10I2N2O3	(M+Na)+
568.8724	1	14634.17	C17H10I2N2O3	(M+Na)+
569.8749	1	1514.81	C17H10I2N2O3	(M+Na)+

--- End Of Report ---

Figure S60. *HRMS of* ***5.***

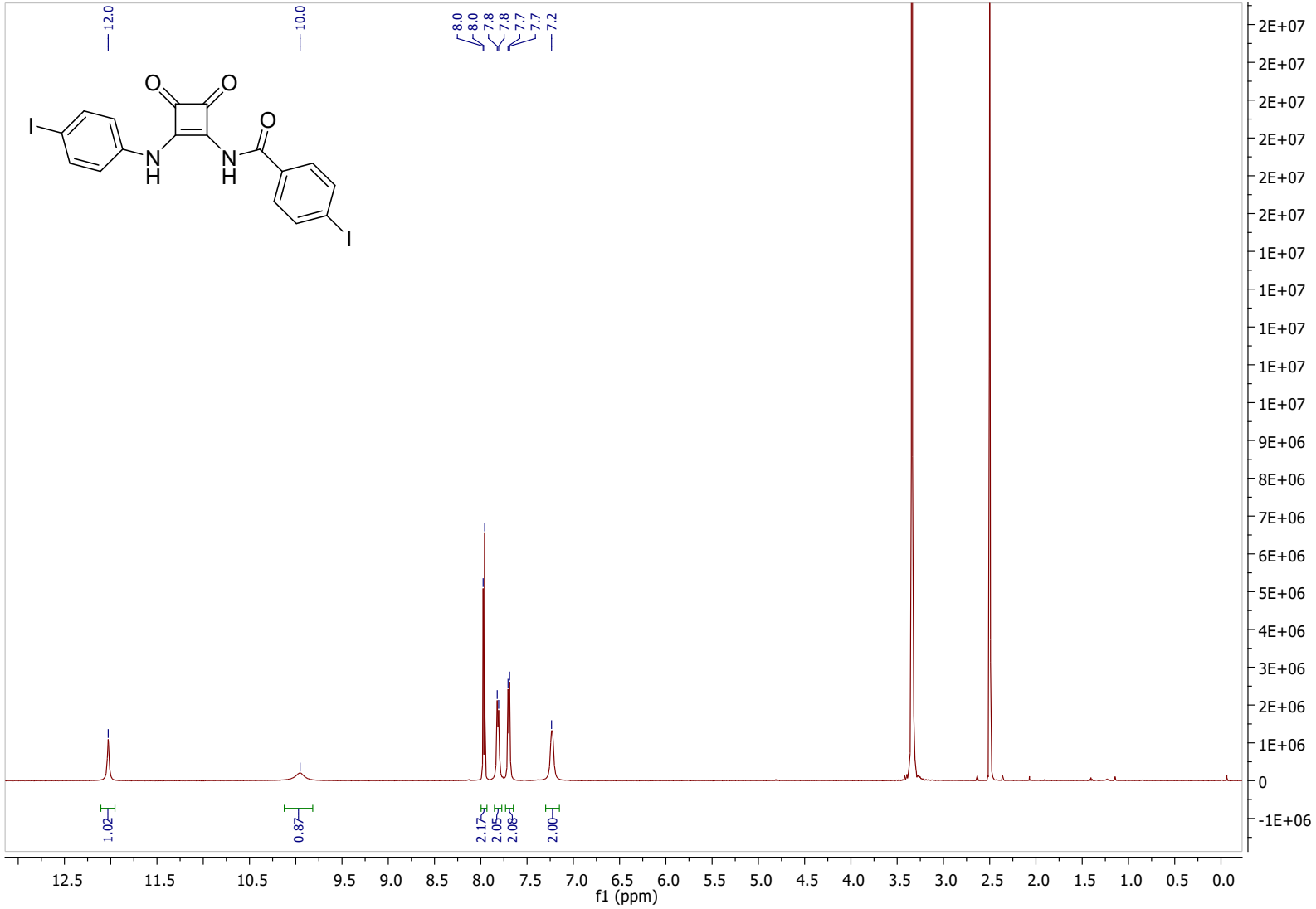


Figure S61. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***6****.*

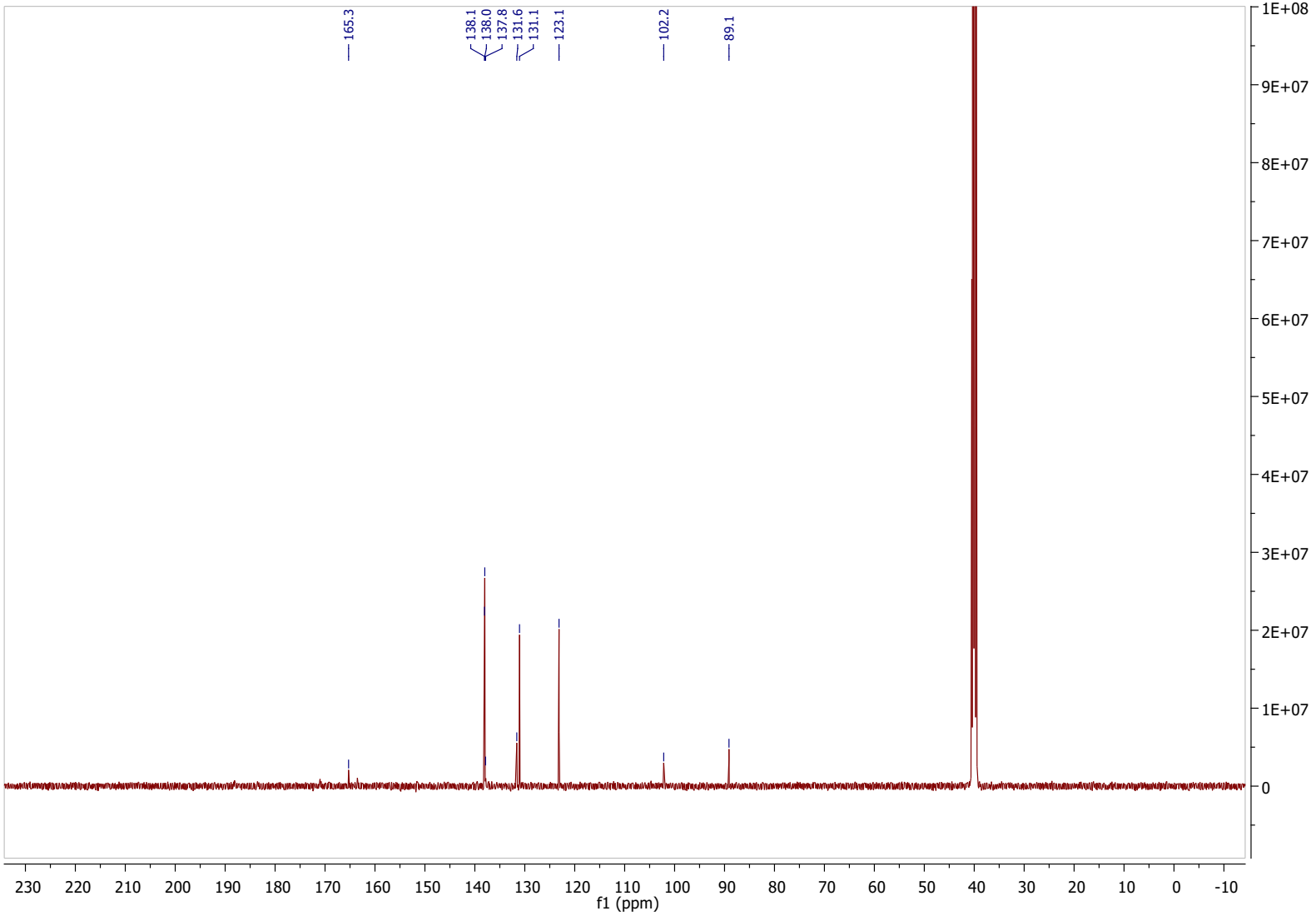


Figure S63. ^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of **6**.

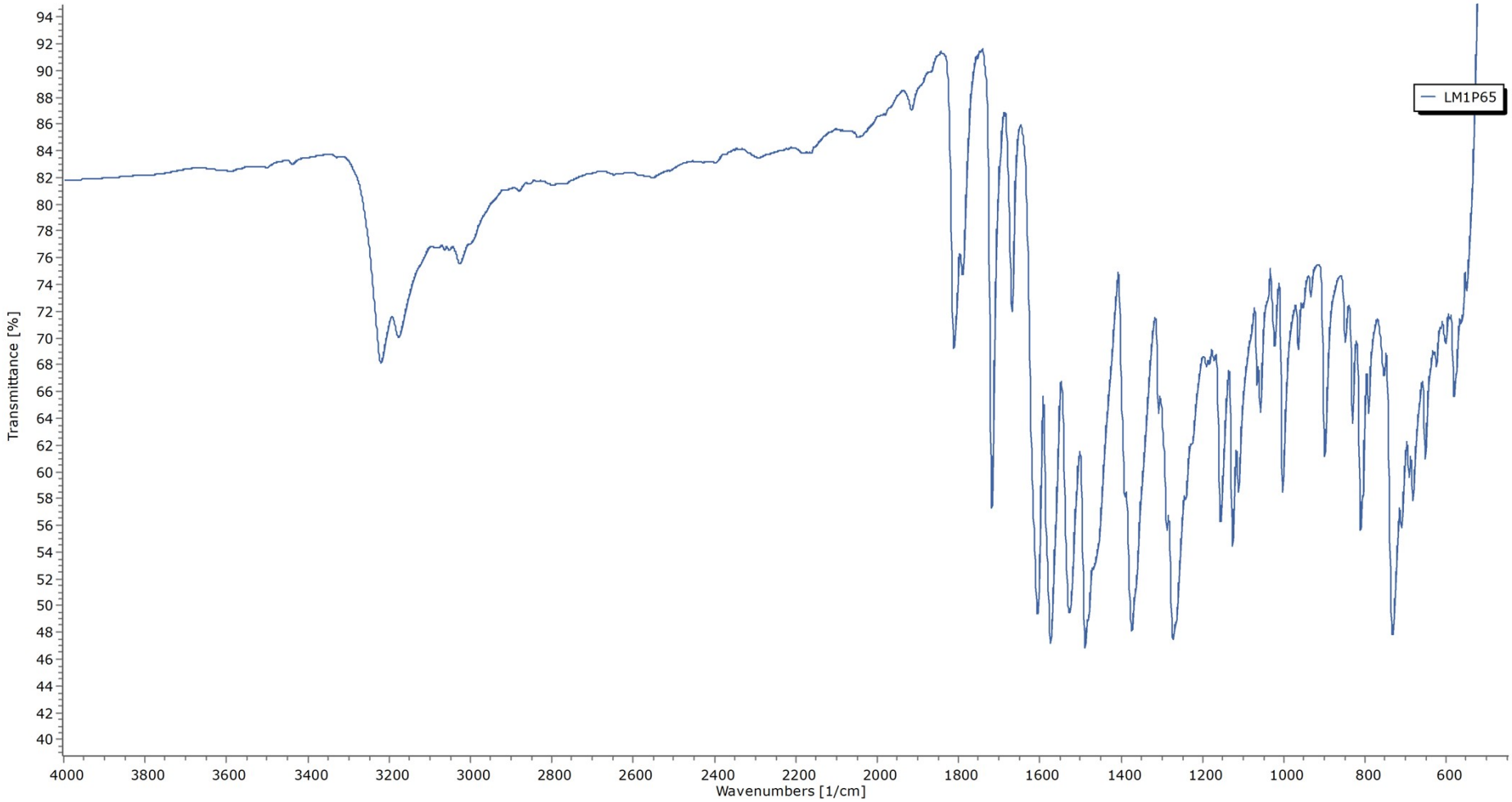
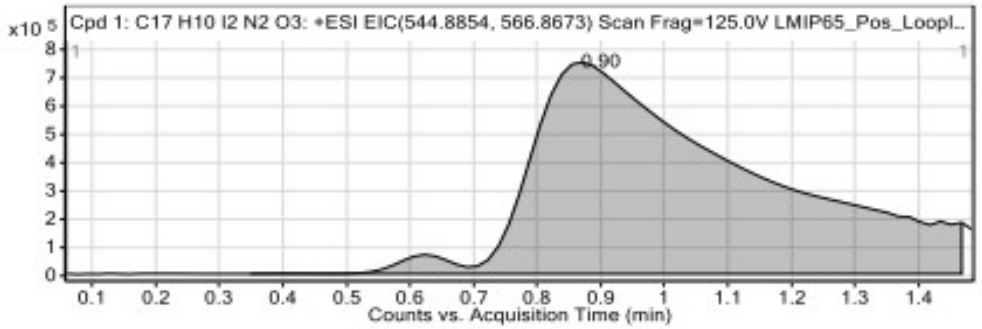


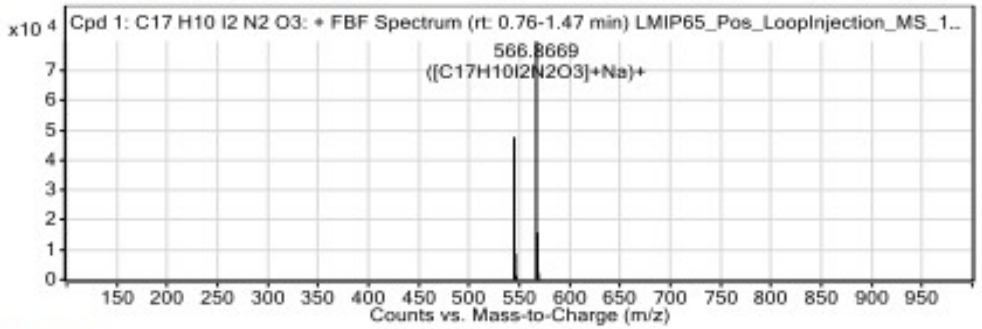
Figure S64. *IR spectrum of* ***6.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.35	0.9	1.47	742996	17890863



Peak List

m/z	z	Abund	Formula	Ion
544.8846	1	47712.78	C17H10I2N2O3	(M+H)+
545.8878	1	8701.18	C17H10I2N2O3	(M+H)+
546.8899	1	1333.92	C17H10I2N2O3	(M+H)+
547.8885	1	163.43	C17H10I2N2O3	(M+H)+
566.8669	1	79898.44	C17H10I2N2O3	(M+Na)+
567.8698	1	15761.88	C17H10I2N2O3	(M+Na)+
568.8725	1	2281.32	C17H10I2N2O3	(M+Na)+
569.8507	1	322.66	C17H10I2N2O3	(M+Na)+

--- End Of Report ---

Figure S65. *HRMS of* ***6.***

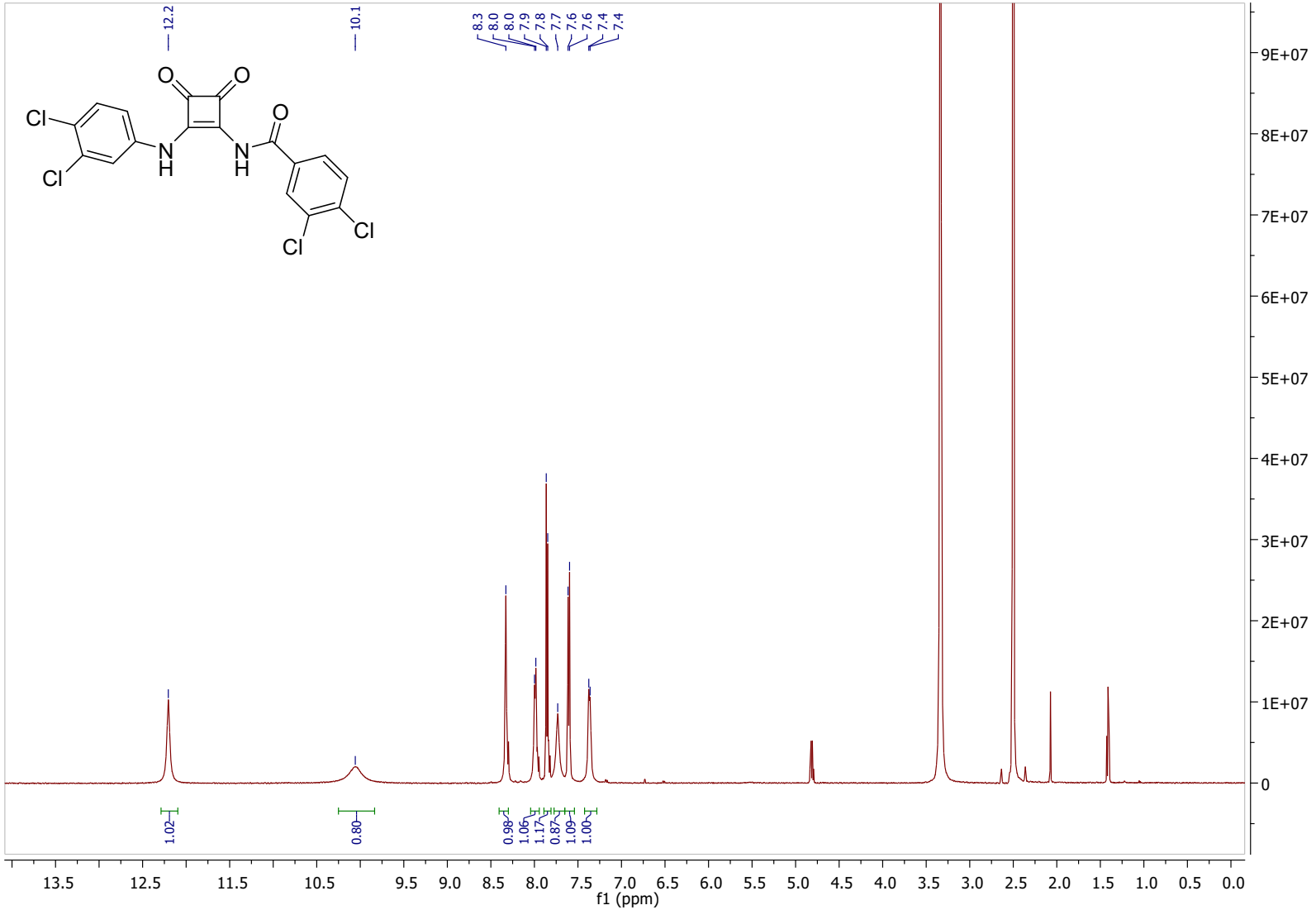


Figure S66. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of **7**.*

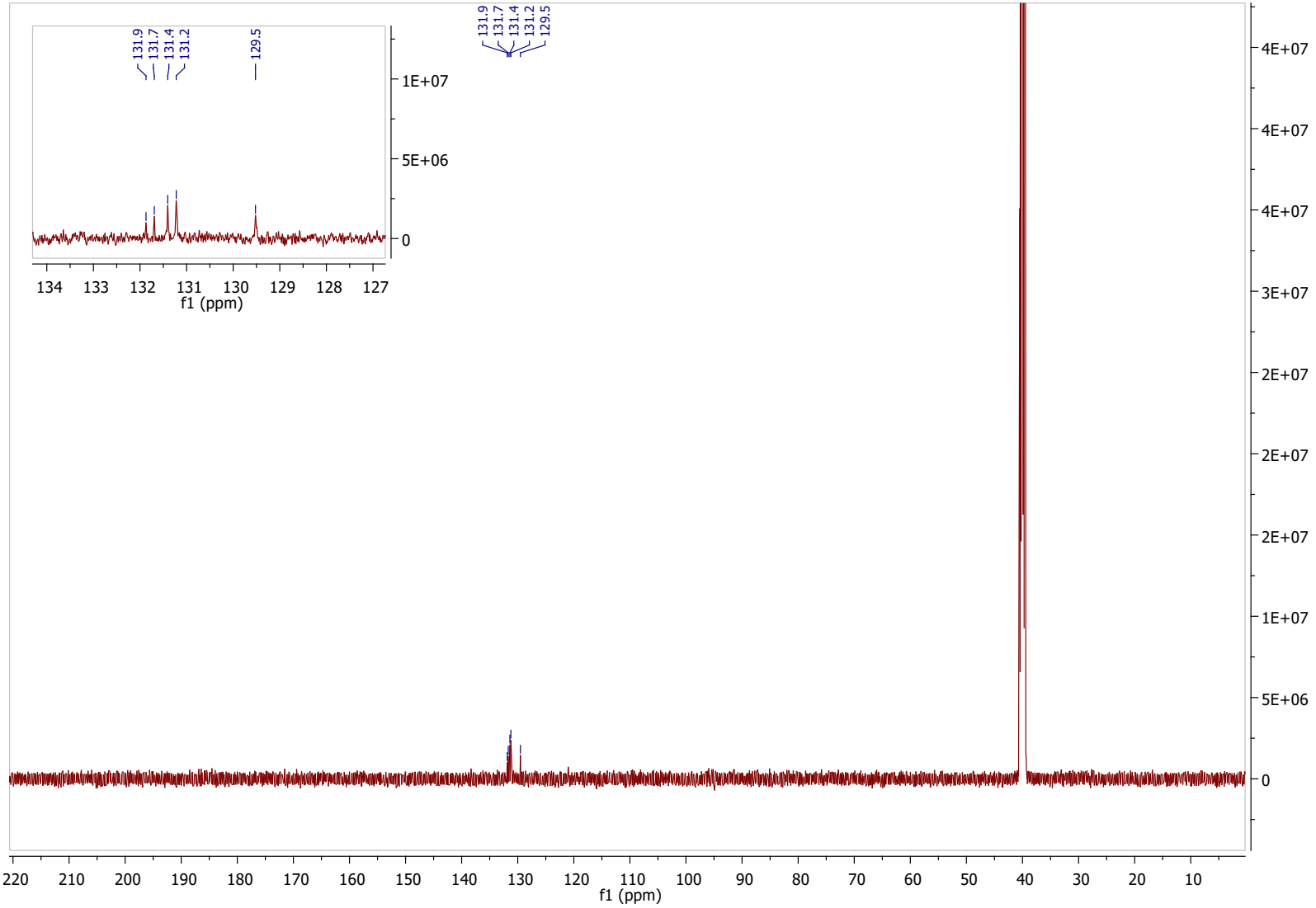


Figure S67. *^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of **7**.*

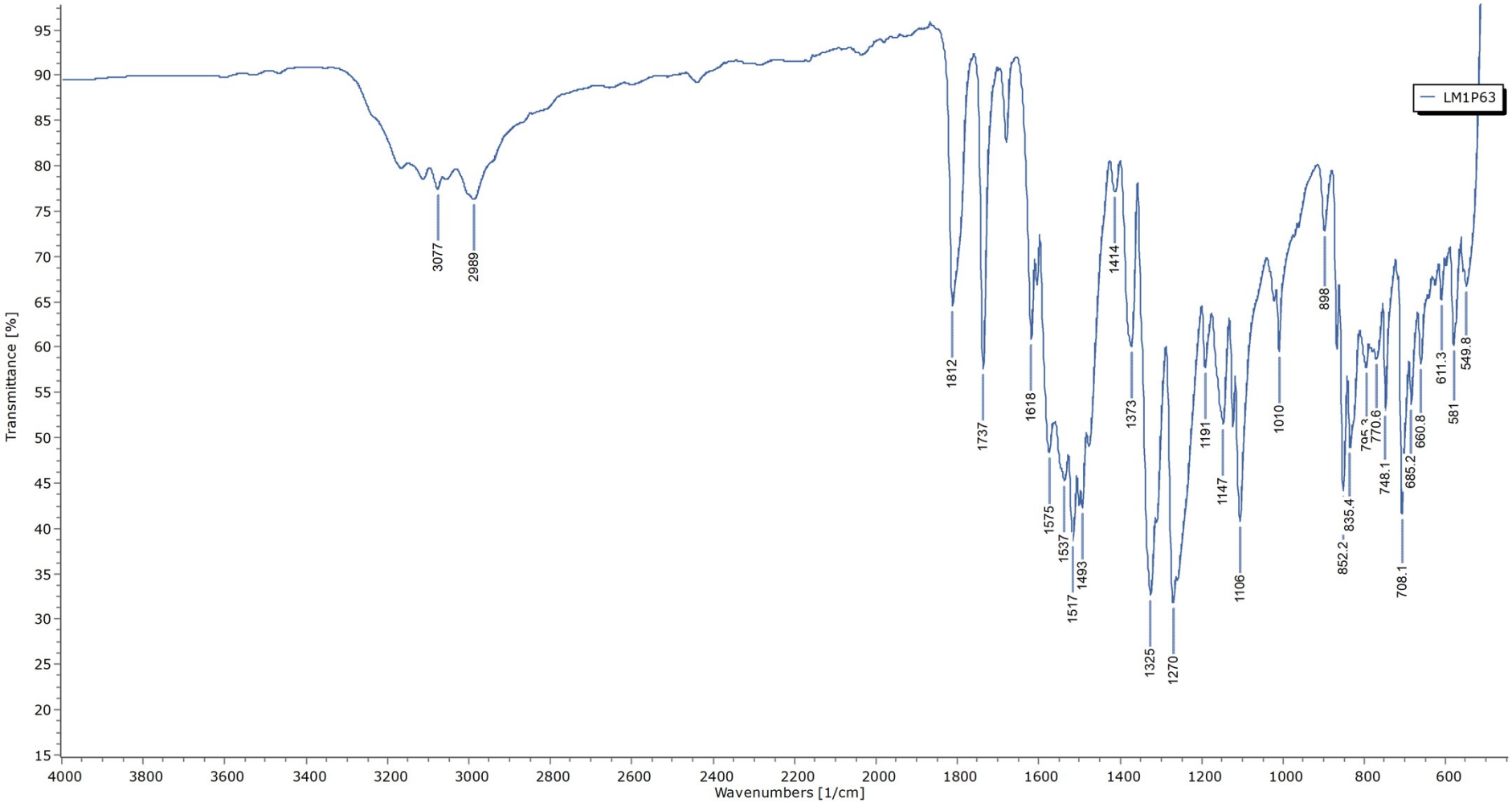
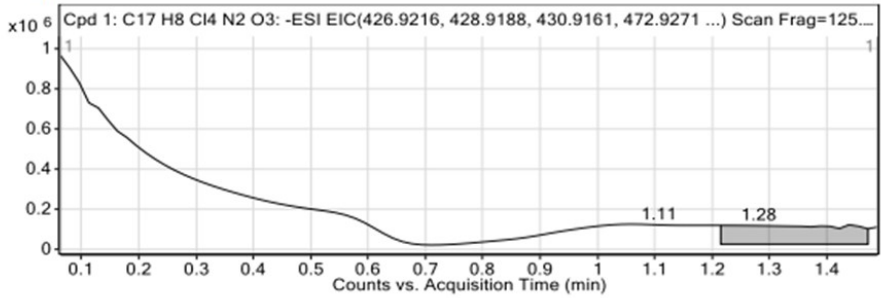


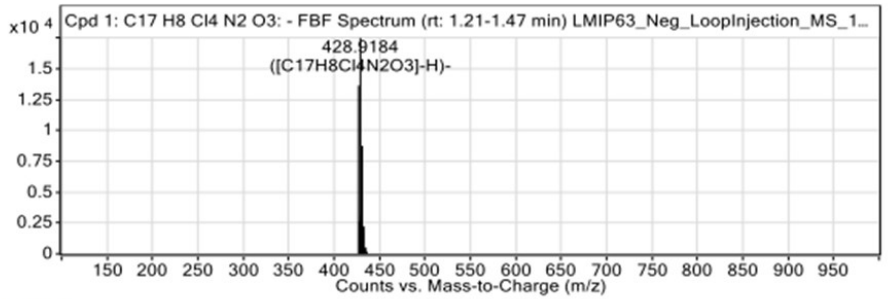
Figure S68. IR spectrum of **7.**

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.75	1.11	1.22	98506	1811788
1.22	1.28	1.47	91992	1385531



Peak List

m/z	z	Abund	Formula	Ion
426.9213	1	13656.46	C17H8Cl4N2O3	(M-H)-
427.9245	1	2656.83	C17H8Cl4N2O3	(M-H)-
428.9184	1	17543.08	C17H8Cl4N2O3	(M-H)-
429.9218	1	3160.57	C17H8Cl4N2O3	(M-H)-
430.9172	1	8763.45	C17H8Cl4N2O3	(M-H)-
431.92	1	1753.84	C17H8Cl4N2O3	(M-H)-
432.9138	1	2221.39	C17H8Cl4N2O3	(M-H)-
433.9161	1	420.11	C17H8Cl4N2O3	(M-H)-
434.8979	1	514.83	C17H8Cl4N2O3	(M-H)-
435.9007	1	176.8	C17H8Cl4N2O3	(M-H)-

--- End Of Report ---

Figure S69. *HRMS of* ***7.***

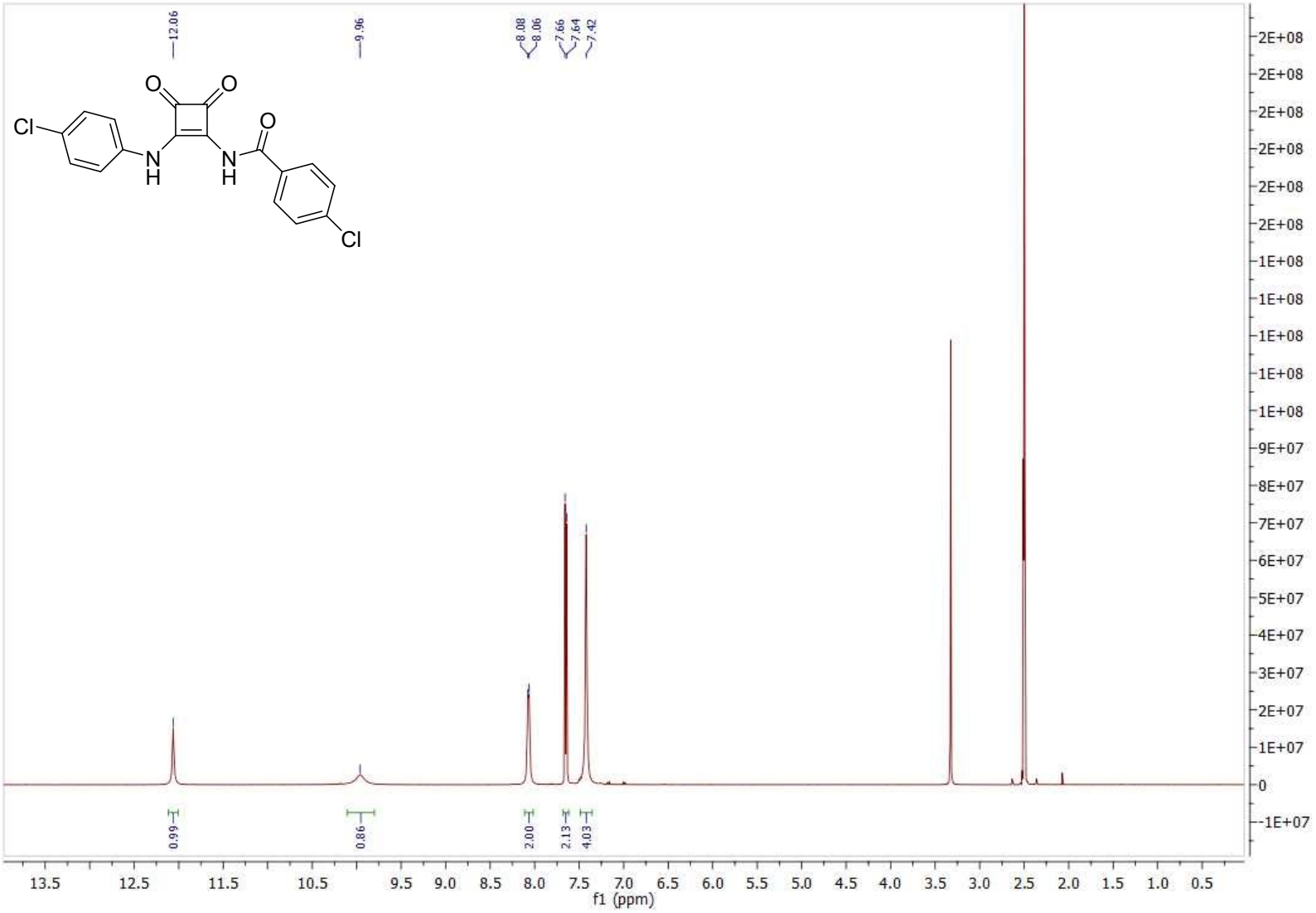


Figure S70. *^{1}H NMR (DMSO-d_6, 500 MHz) spectrum of* ***8****.*

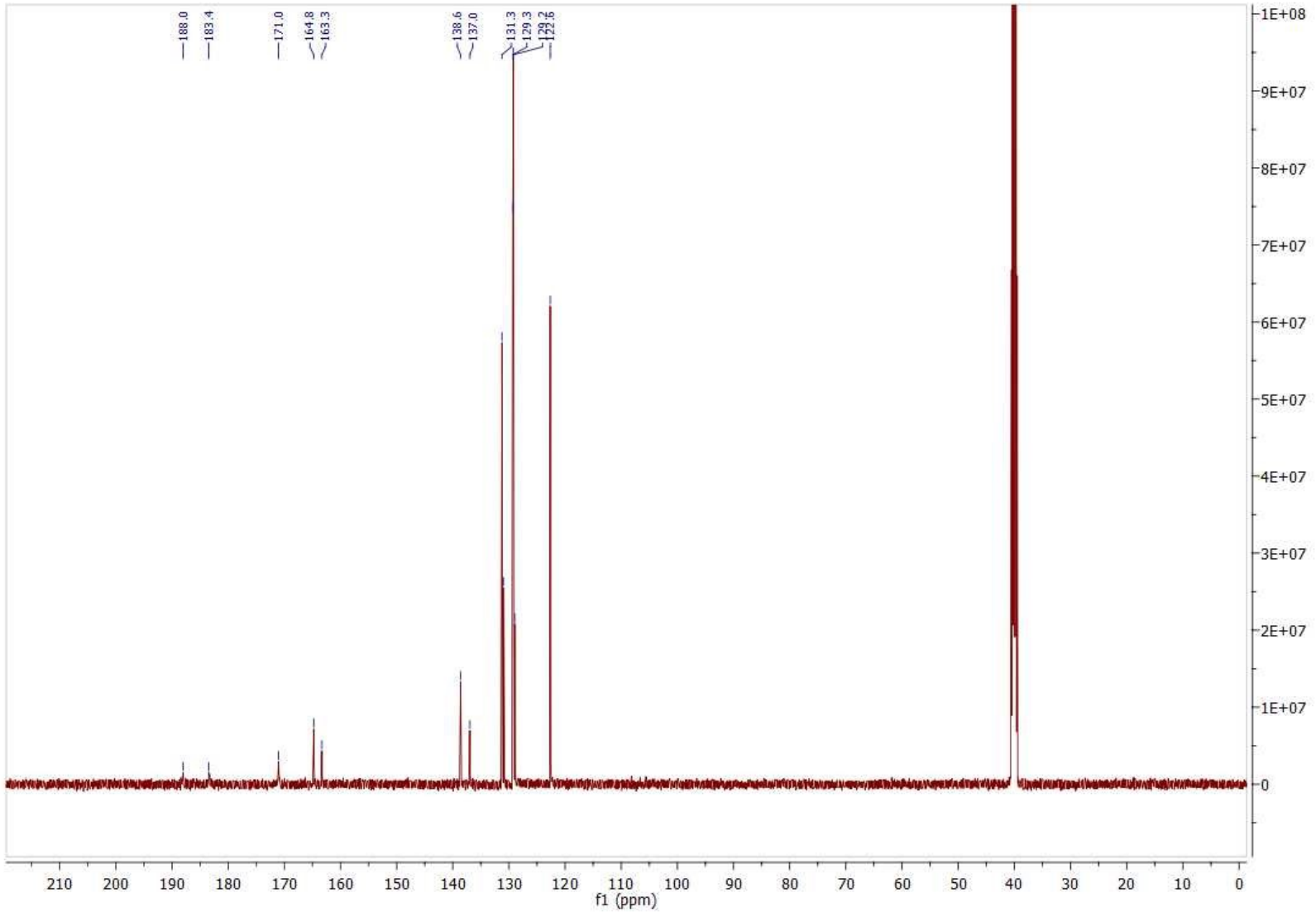


Figure S71. ^{13}C NMR (DMSO-d_6, 126 MHz) spectrum of **8**.

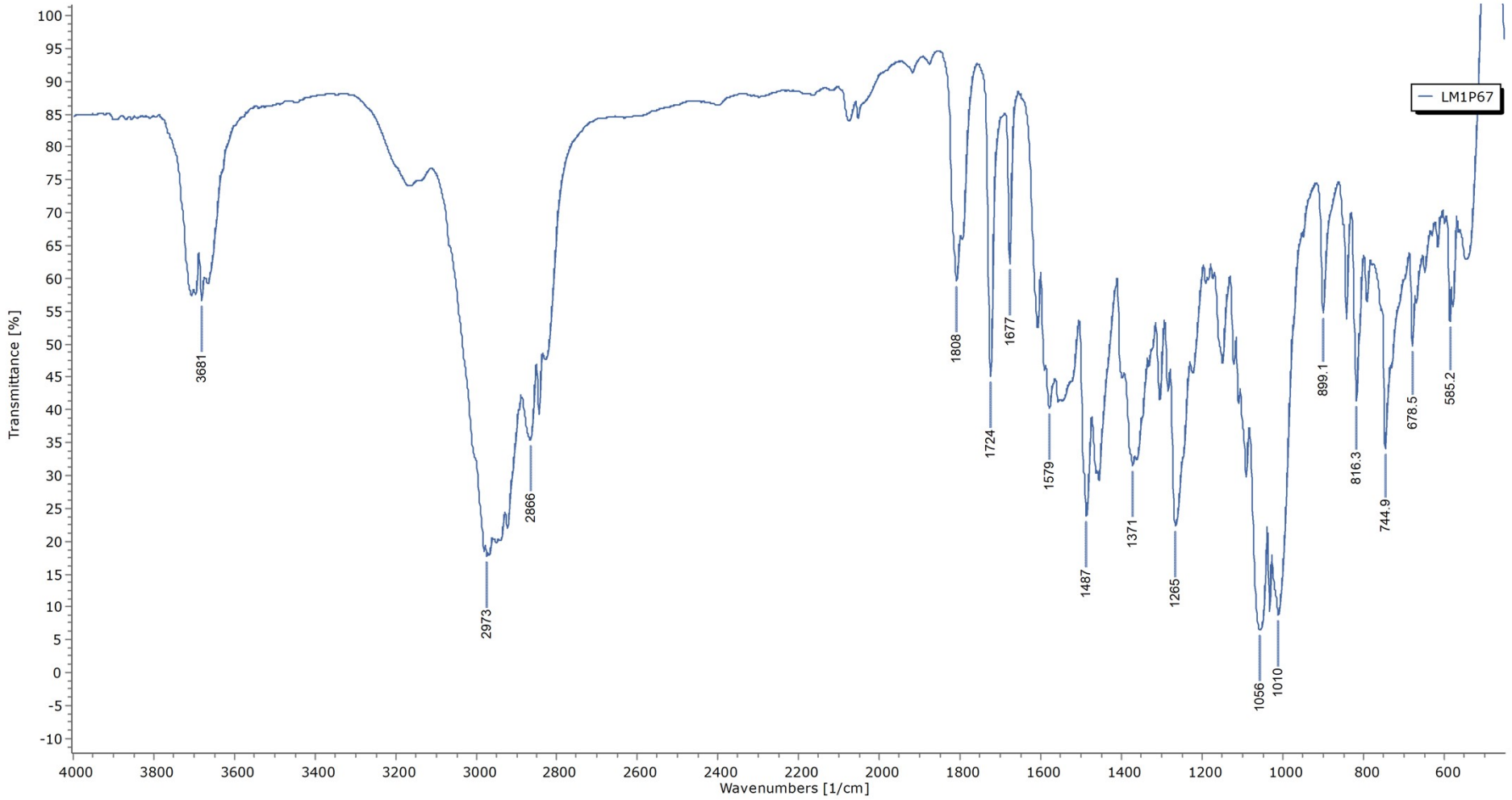
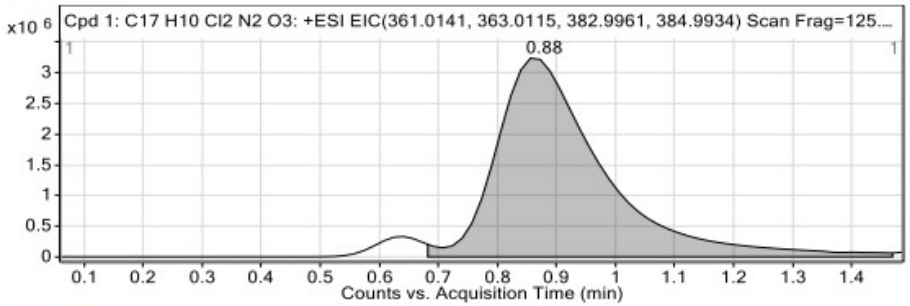


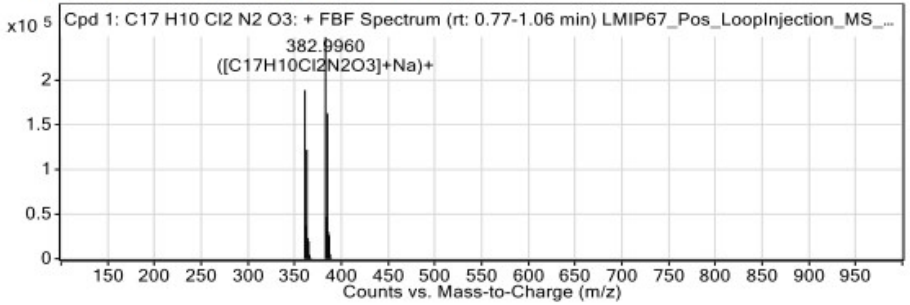
Figure S72. *IR spectrum of* ***8.***

Compounds



Integration Peak List

Start	RT	End	Height	Area
0.68	0.88	1.47	3052489	40426406



Peak List

m/z	z	Abund	Formula	Ion
361.014	1	188503.16	C17H10Cl2N2O3	(M+H)+
362.0172	1	37399.45	C17H10Cl2N2O3	(M+H)+
363.0113	1	121920.34	C17H10Cl2N2O3	(M+H)+
364.0142	1	23217.99	C17H10Cl2N2O3	(M+H)+
365.009	1	19490.81	C17H10Cl2N2O3	(M+H)+
382.996	1	248171.25	C17H10Cl2N2O3	(M+Na)+
383.9989	1	47022.43	C17H10Cl2N2O3	(M+Na)+
384.9934	1	162578.2	C17H10Cl2N2O3	(M+Na)+
385.9962	1	30132.79	C17H10Cl2N2O3	(M+Na)+
386.991	1	26273.02	C17H10Cl2N2O3	(M+Na)+

--- End Of Report ---

Figure S73. *HRMS of* ***8.***

UV/Vis-Spectrometric pK_a Determination

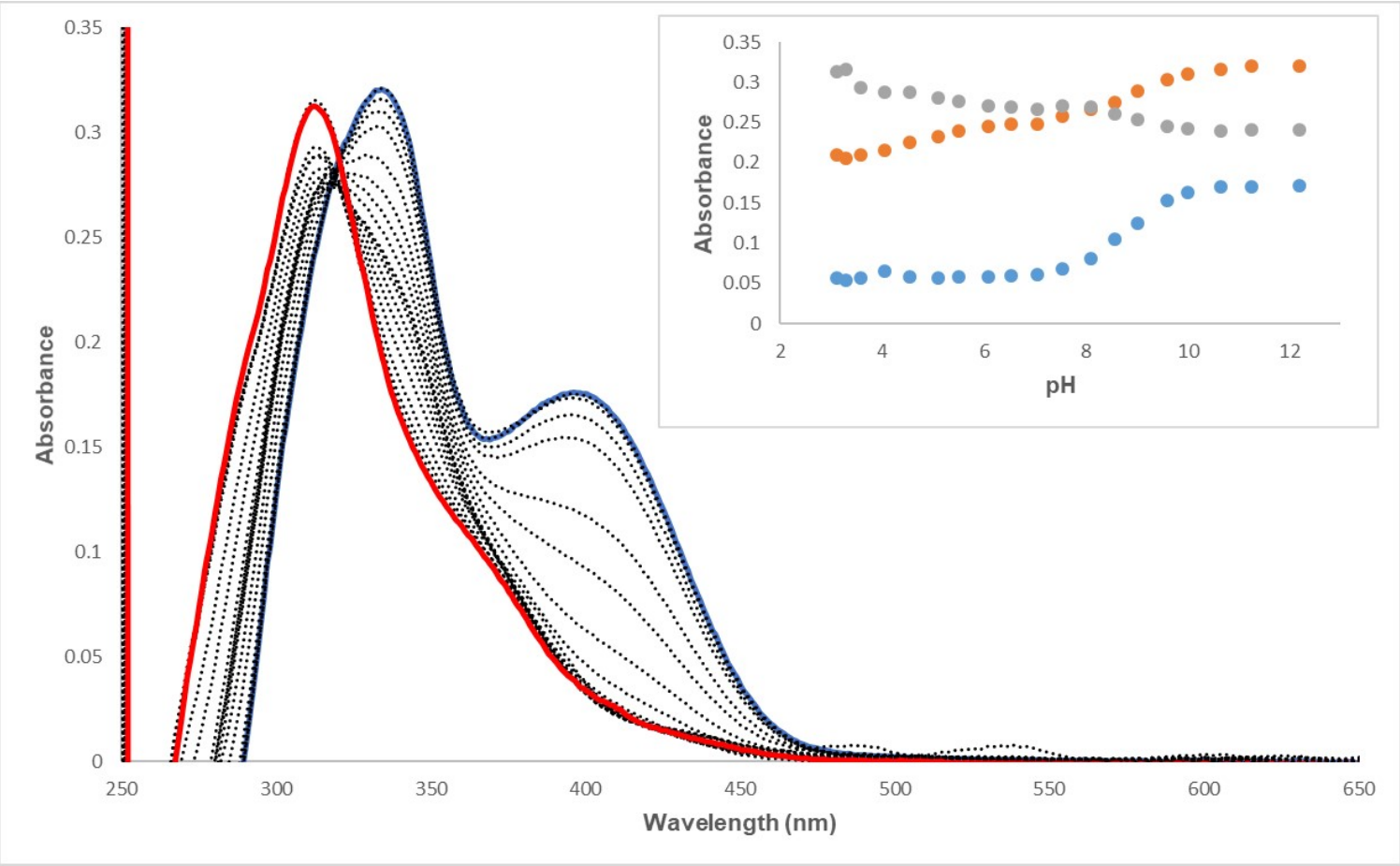


Figure S74. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***1*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 3.29 (red), pH 12.18 (blue). Inset: Comparison plots of absorbance at 312 nm (grey), 332 nm (orange), 312 nm (blue) vs. pH.*

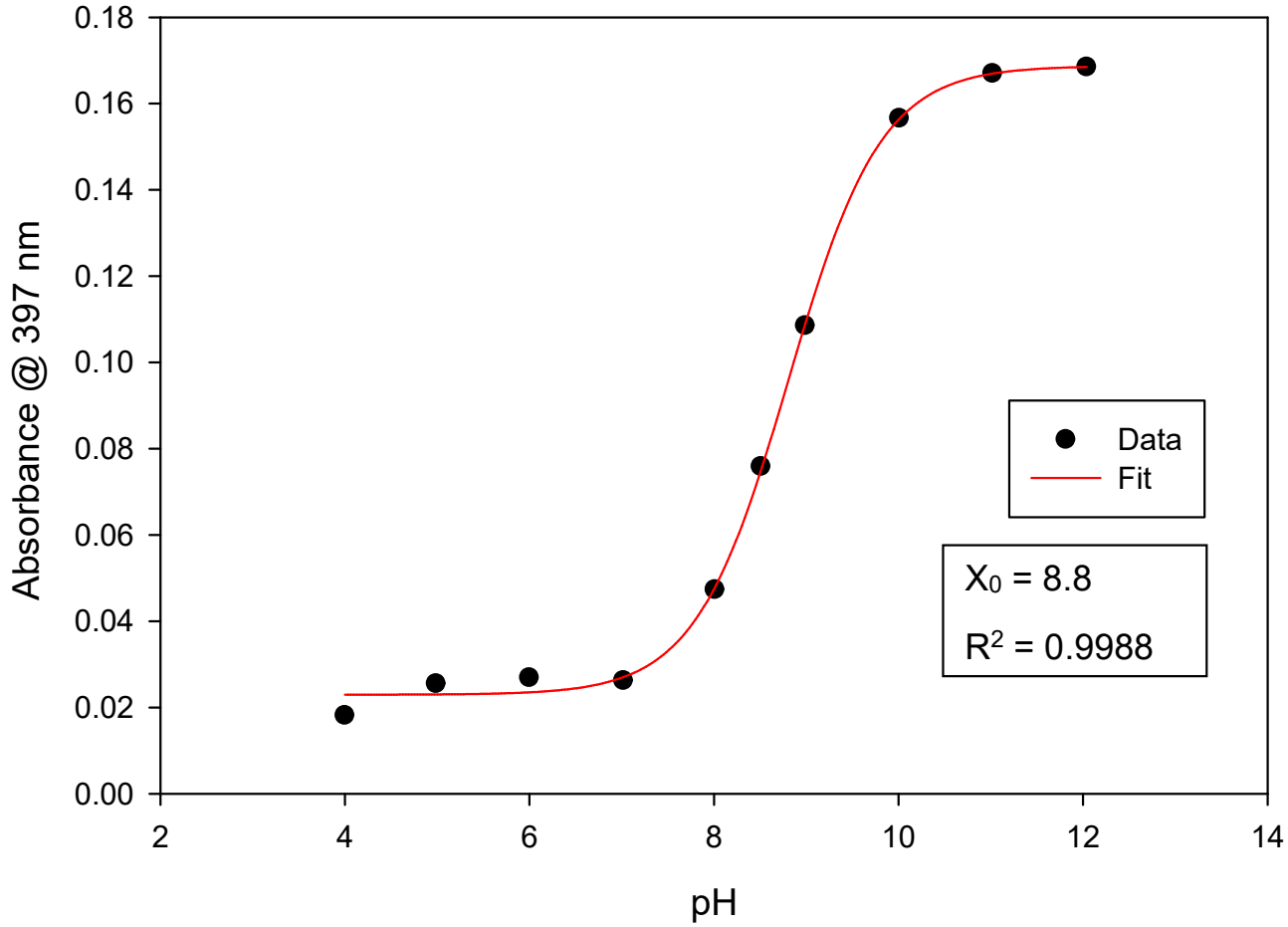


Figure S75. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***1.***

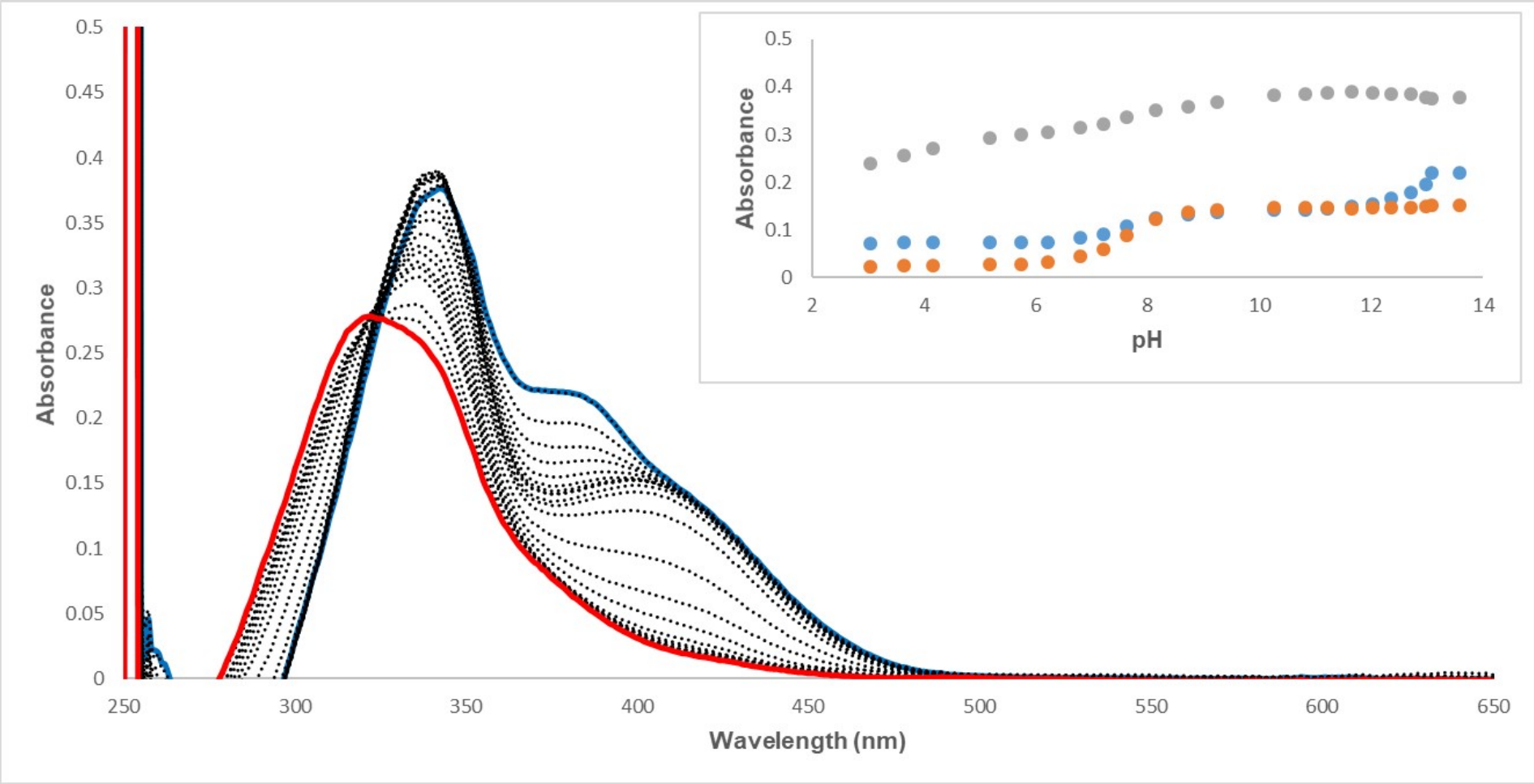


Figure S76. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***2*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 3.04 (red), pH 13.08 (blue). Inset: Comparison plots of absorbance at 342 nm (grey), 410 nm (orange), 378 nm (blue) vs. pH.*

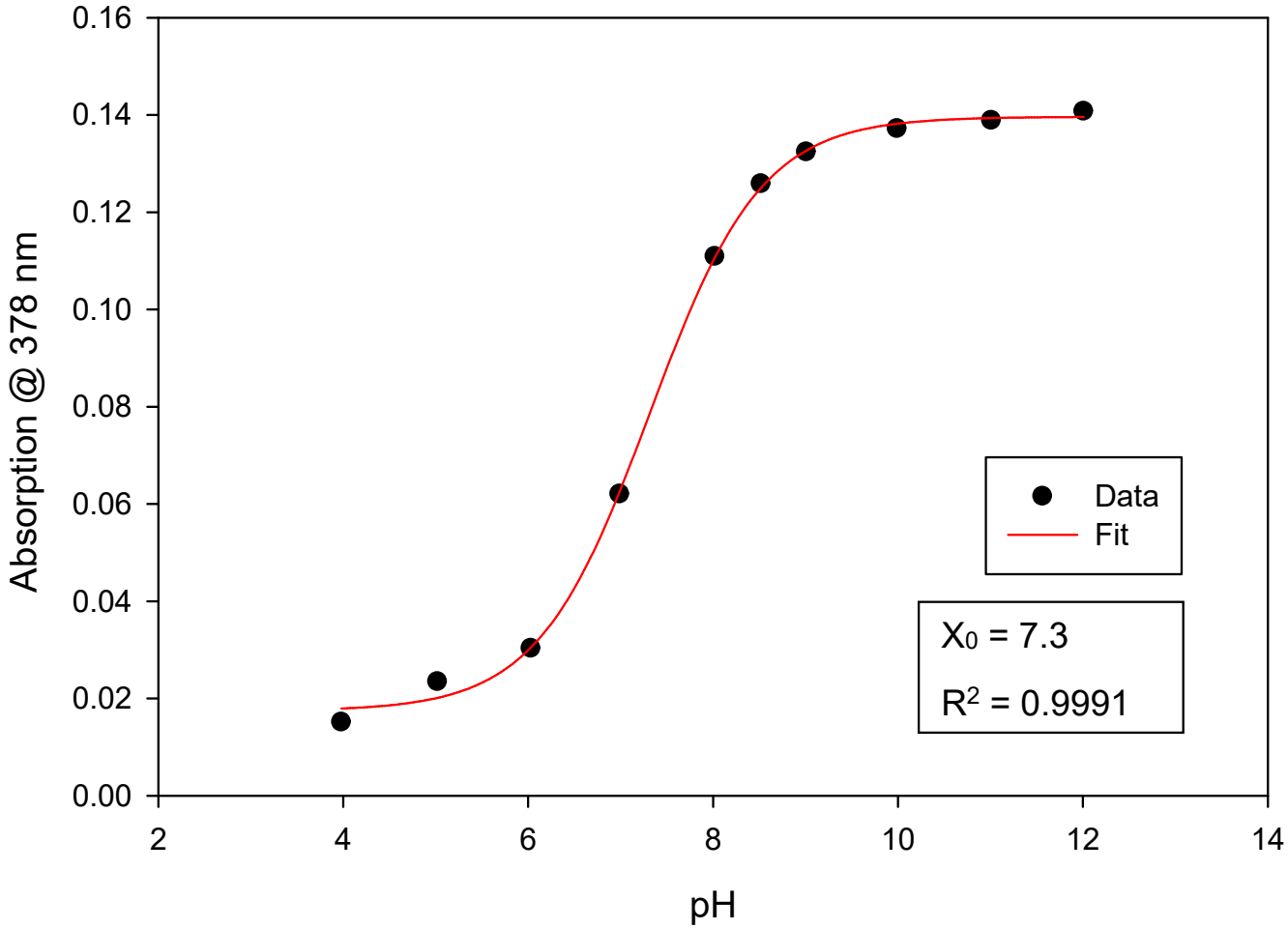


Figure S77. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***2.***

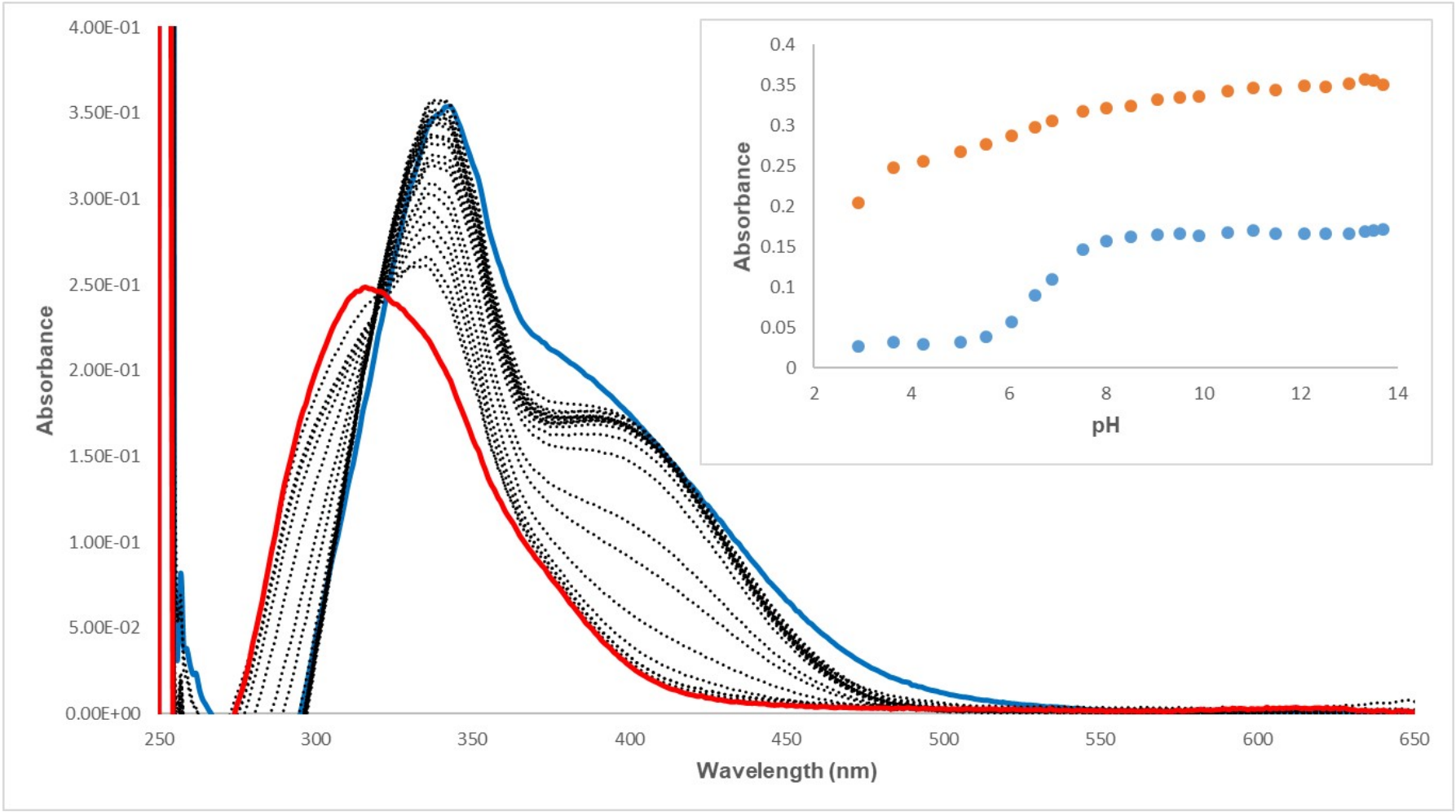


Figure S78. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***3*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 2.90 (red), pH 12.46 (blue). Inset: Comparison plots of absorbance at 340 nm (orange) and 401 nm (blue) vs. pH.*

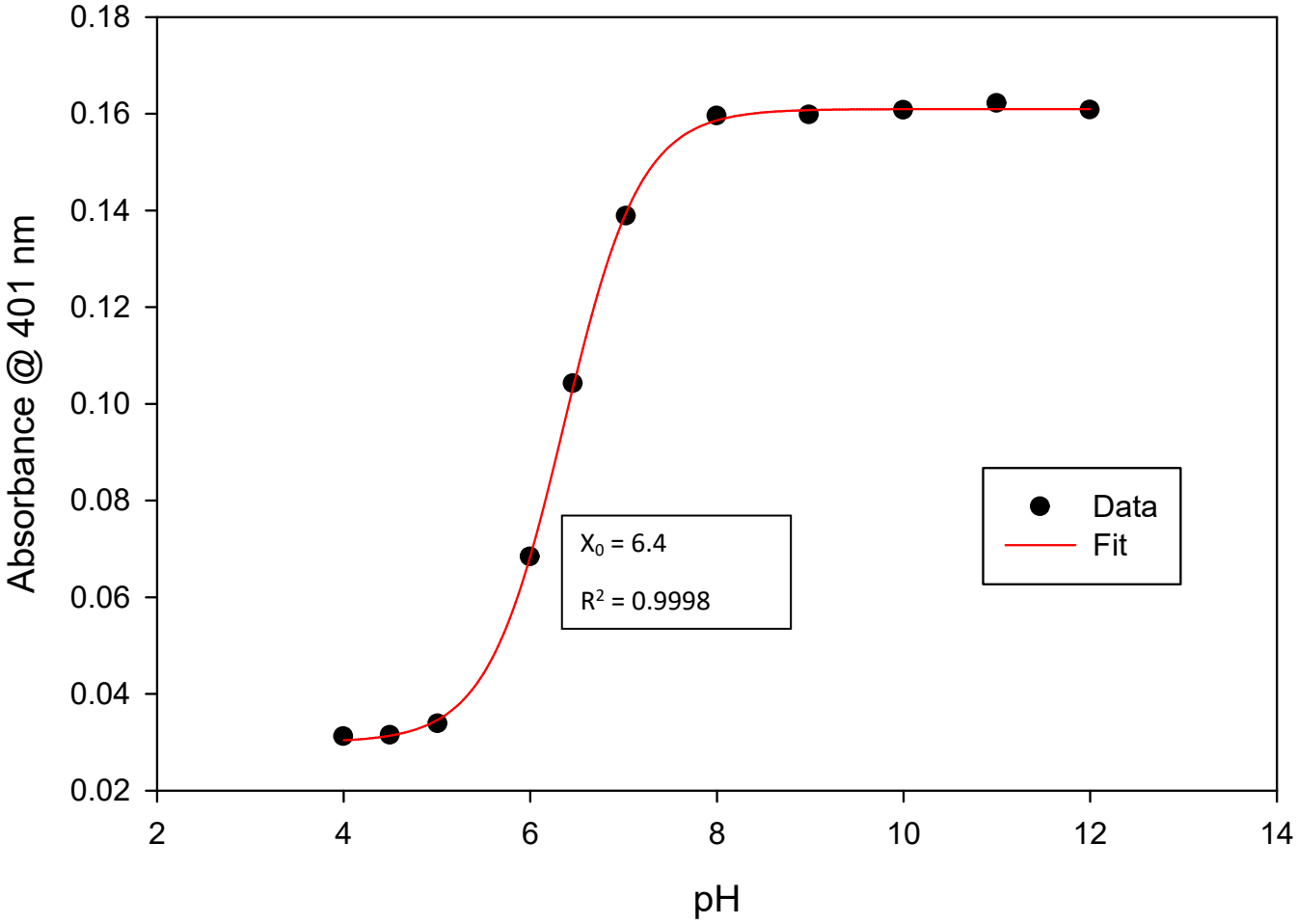


Figure S79. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***3****.*

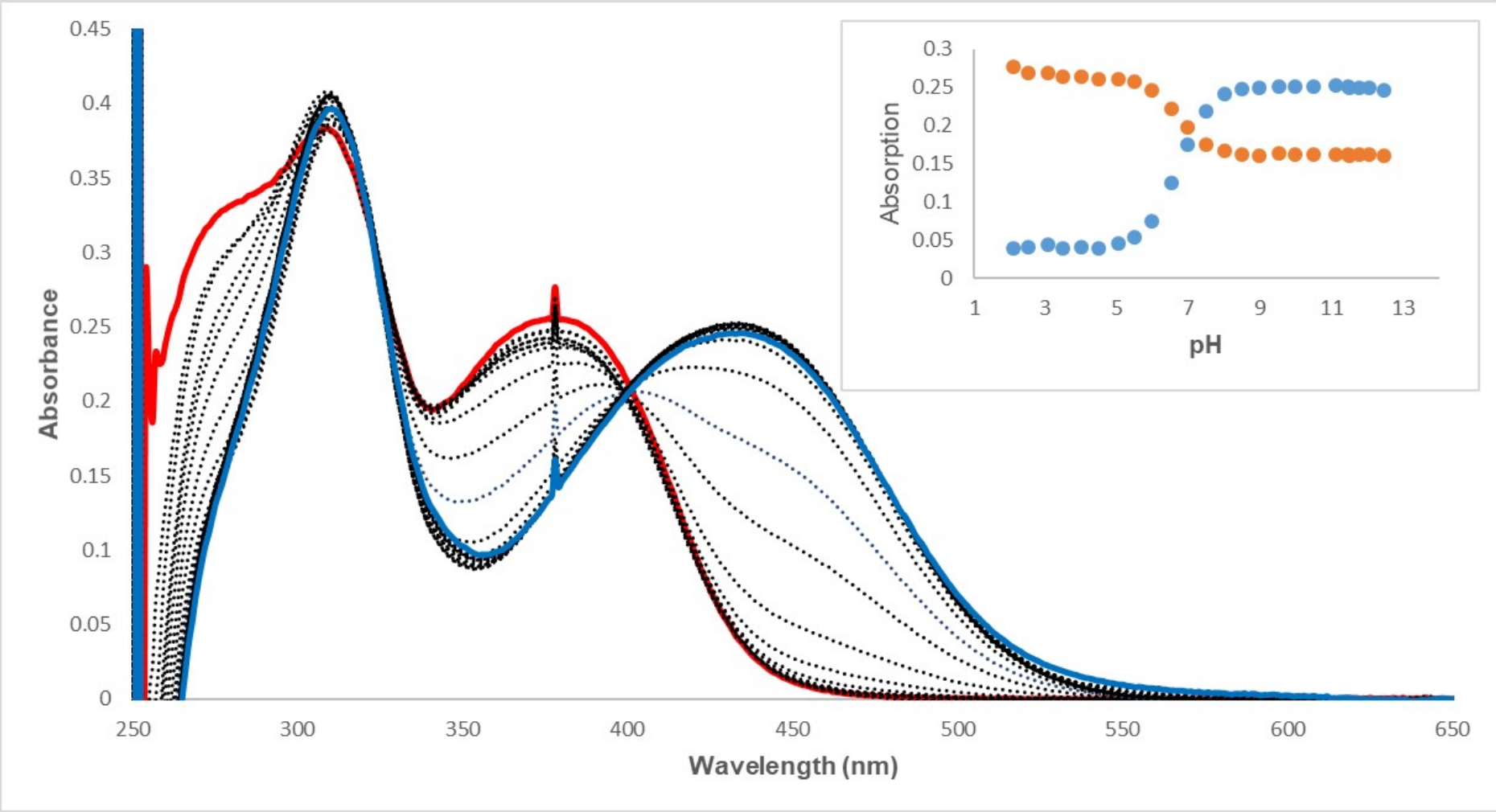


Figure S80. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***4*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 2.08 (red), pH 13.70 (blue). Inset: Comparison plots of absorbance at 378 nm (orange) and 434 nm (blue) vs. pH.*

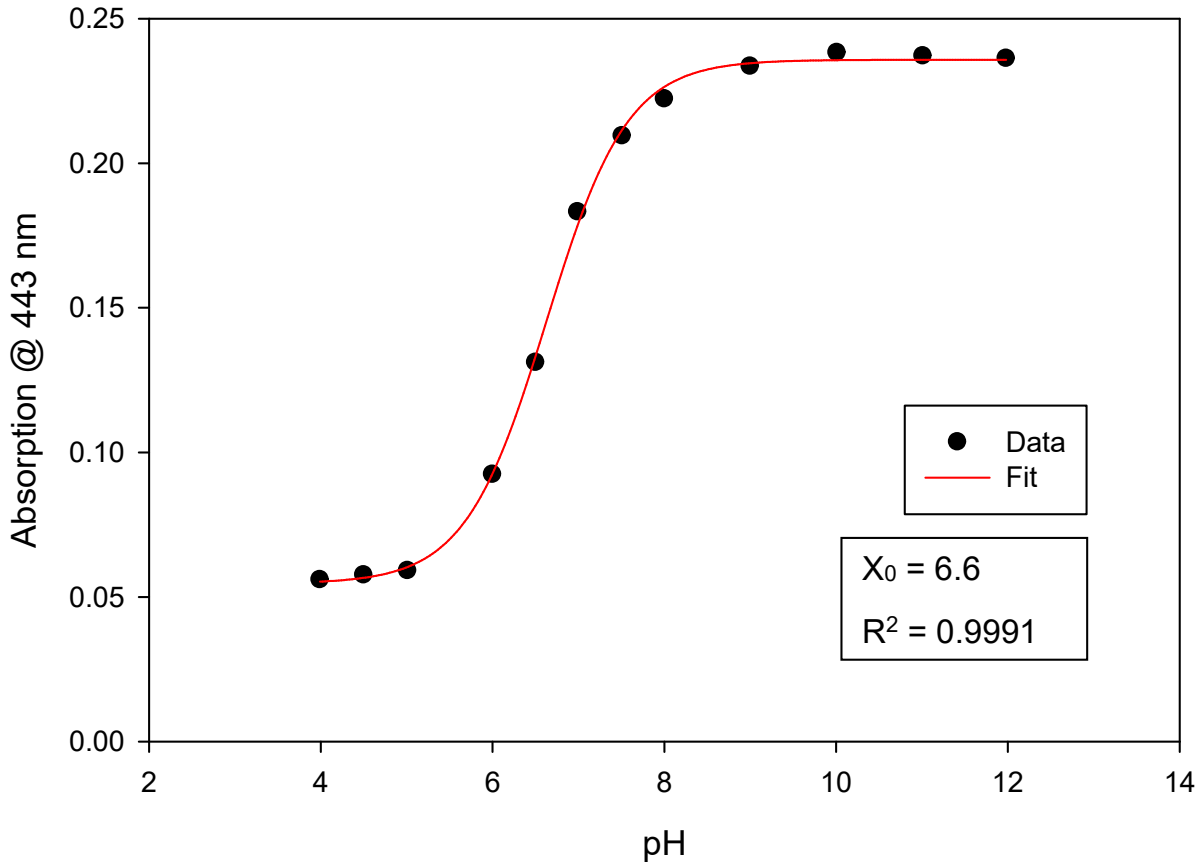


Figure S81. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***4****.*

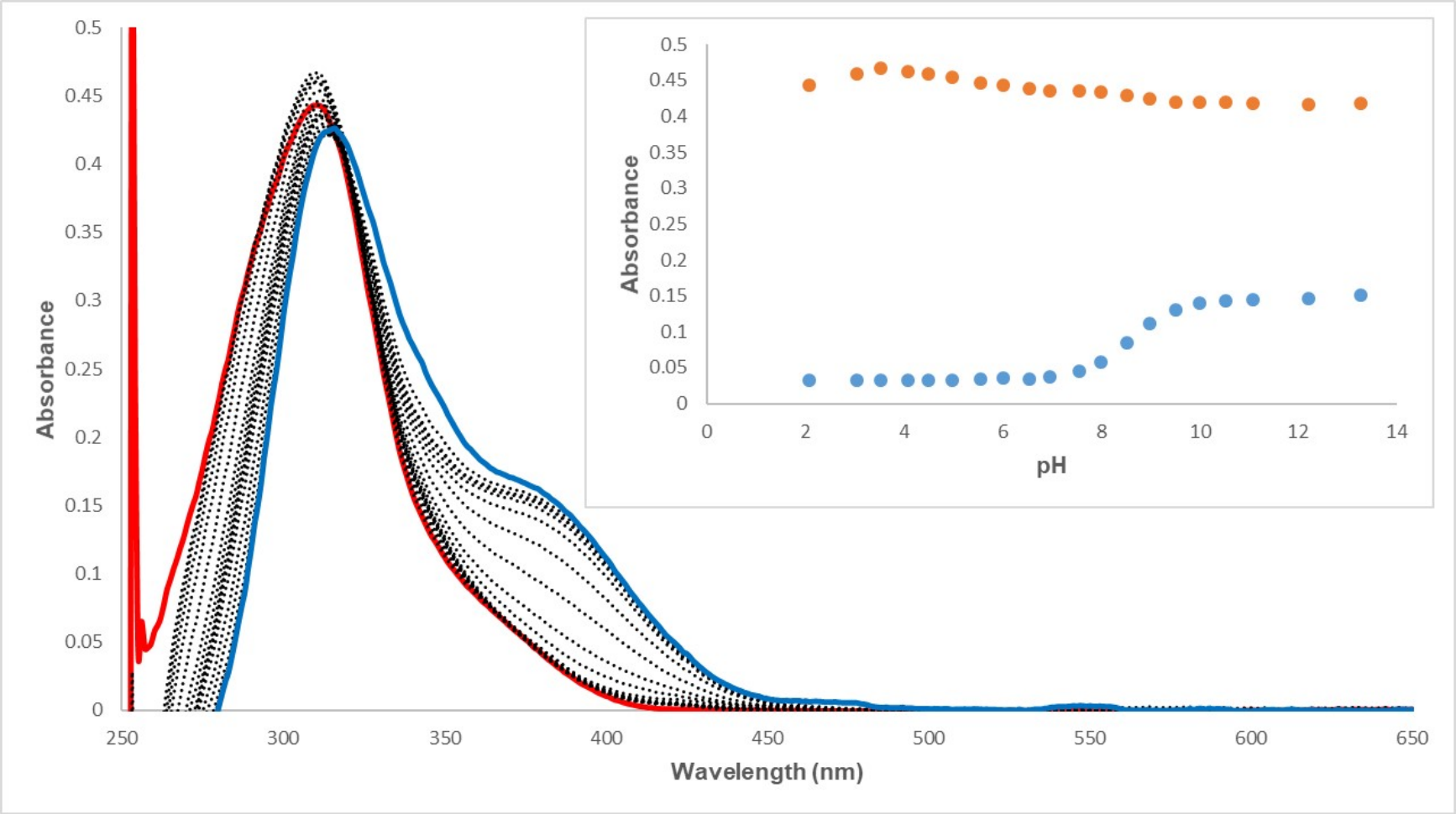


Figure S82. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***5*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 2.08 (red), pH 13.27 (blue). Inset: Comparison plots of absorbance at 311 nm (orange) and 385 nm (blue) vs. pH.*

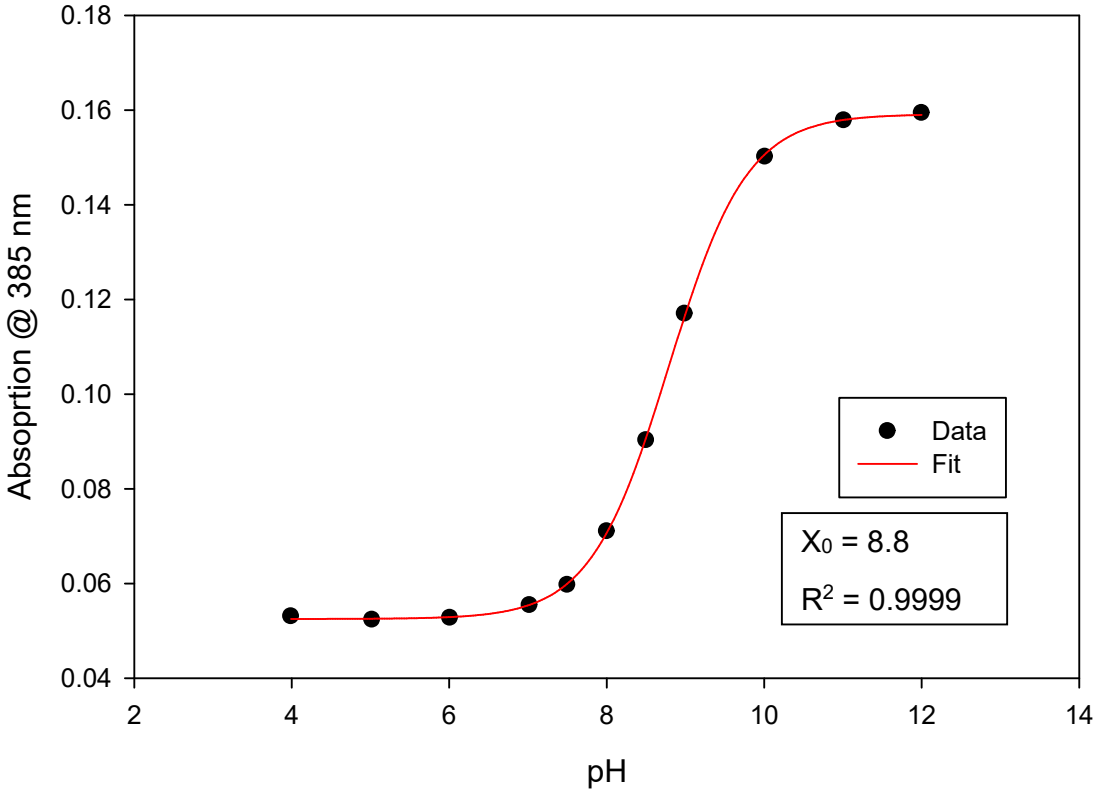


Figure S83. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***5****.*

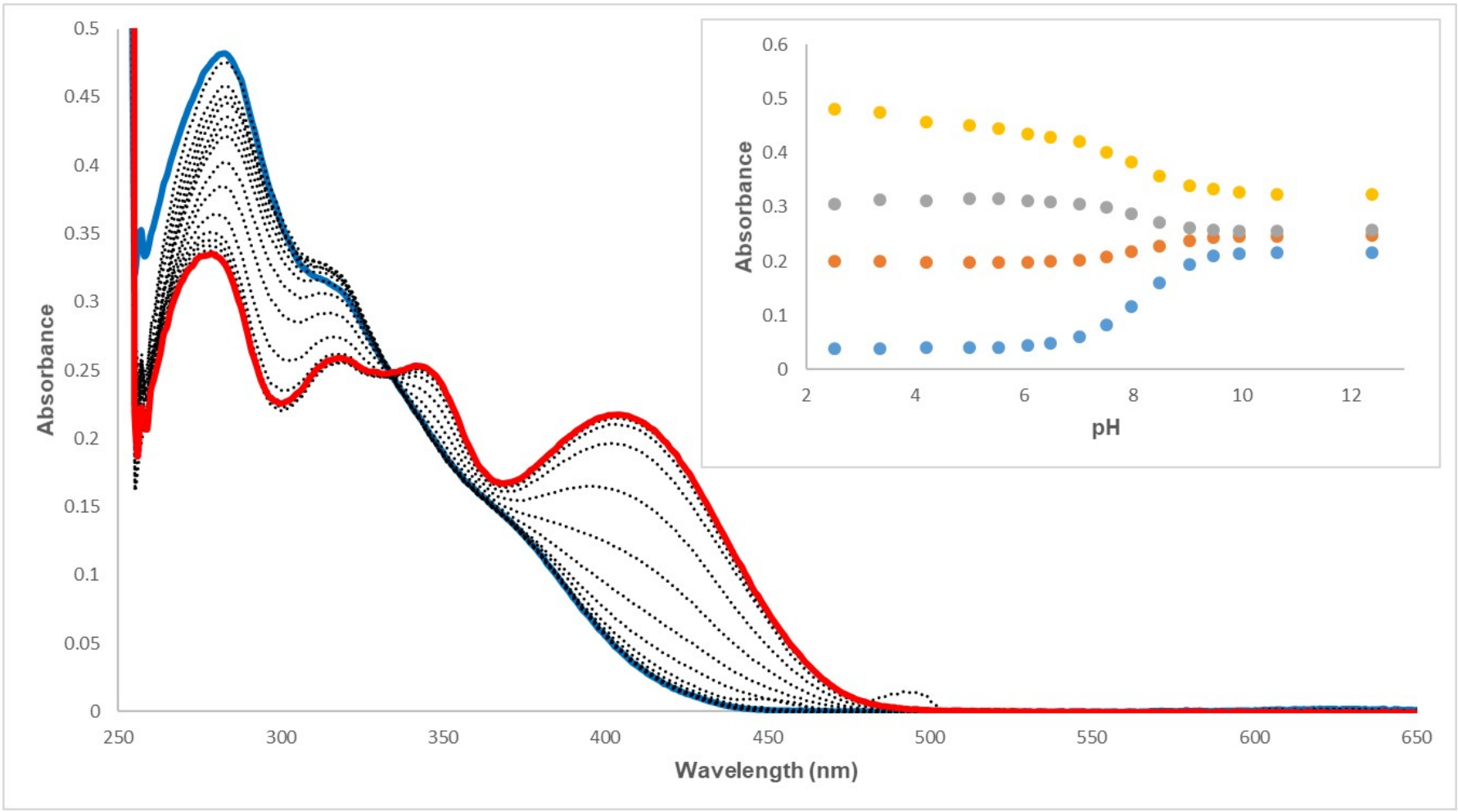


Figure S84. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***6*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 2.52 (red), pH 12.40 (blue). Inset: Comparison plots of absorbance at 284 nm (yellow), 320 nm (grey), 347 nm (orange), and 407 nm (blue) vs. pH.*

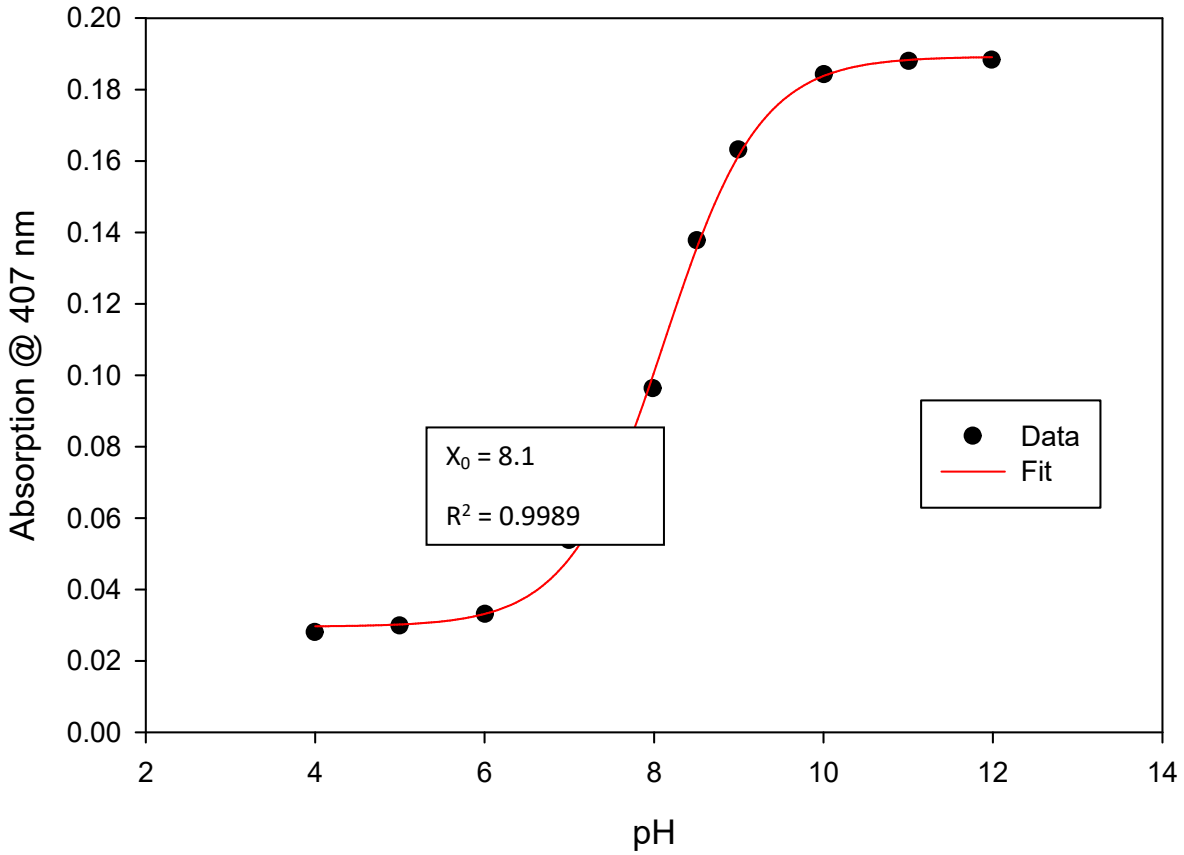


Figure S85. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***6****.*

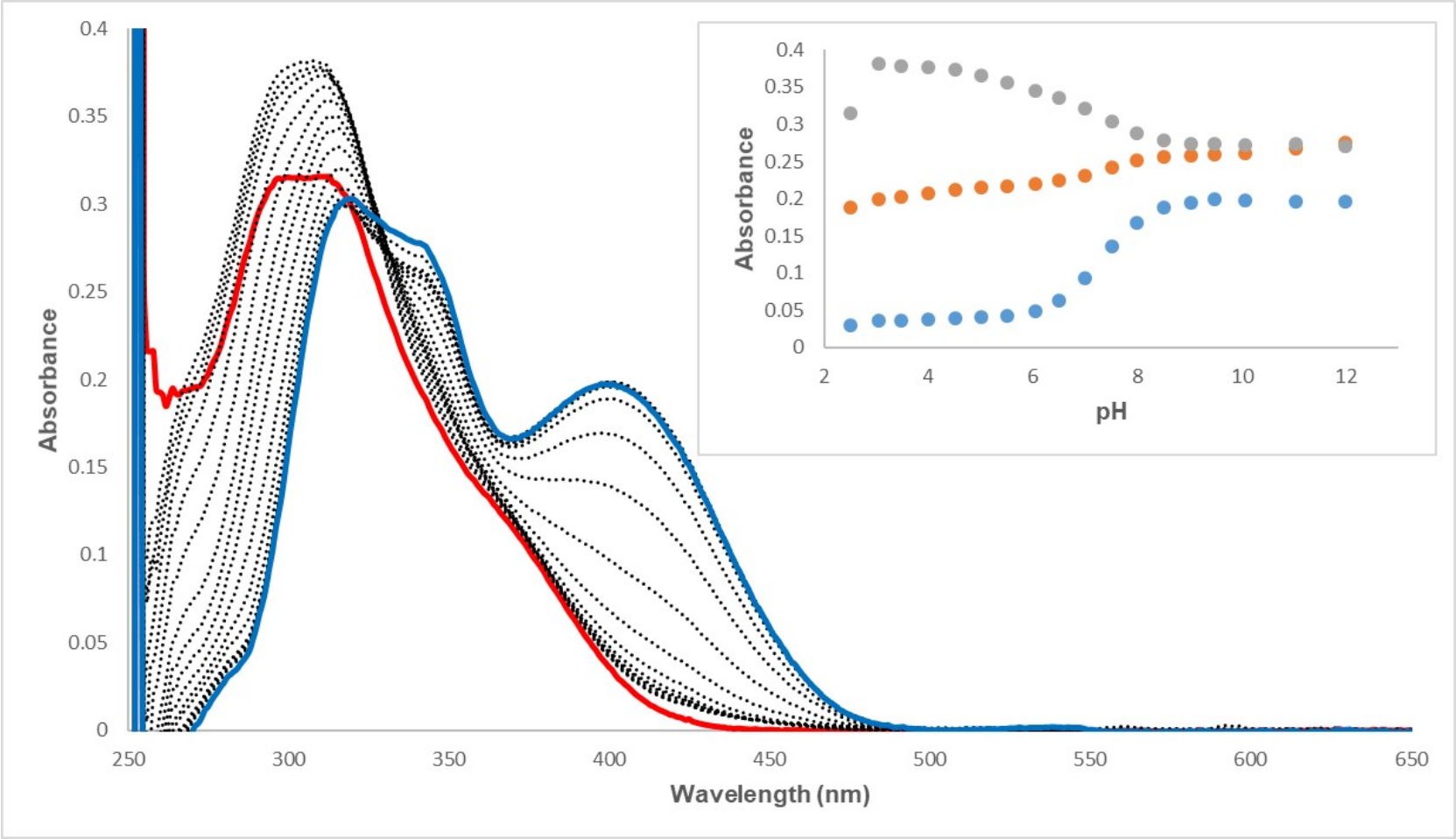


Figure S86. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***7*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 2.50 (red), pH 11.98 (blue). Inset: Comparison plots of absorbance at 310 nm (grey), 343 nm (orange), and 403 nm (blue) vs. pH.*

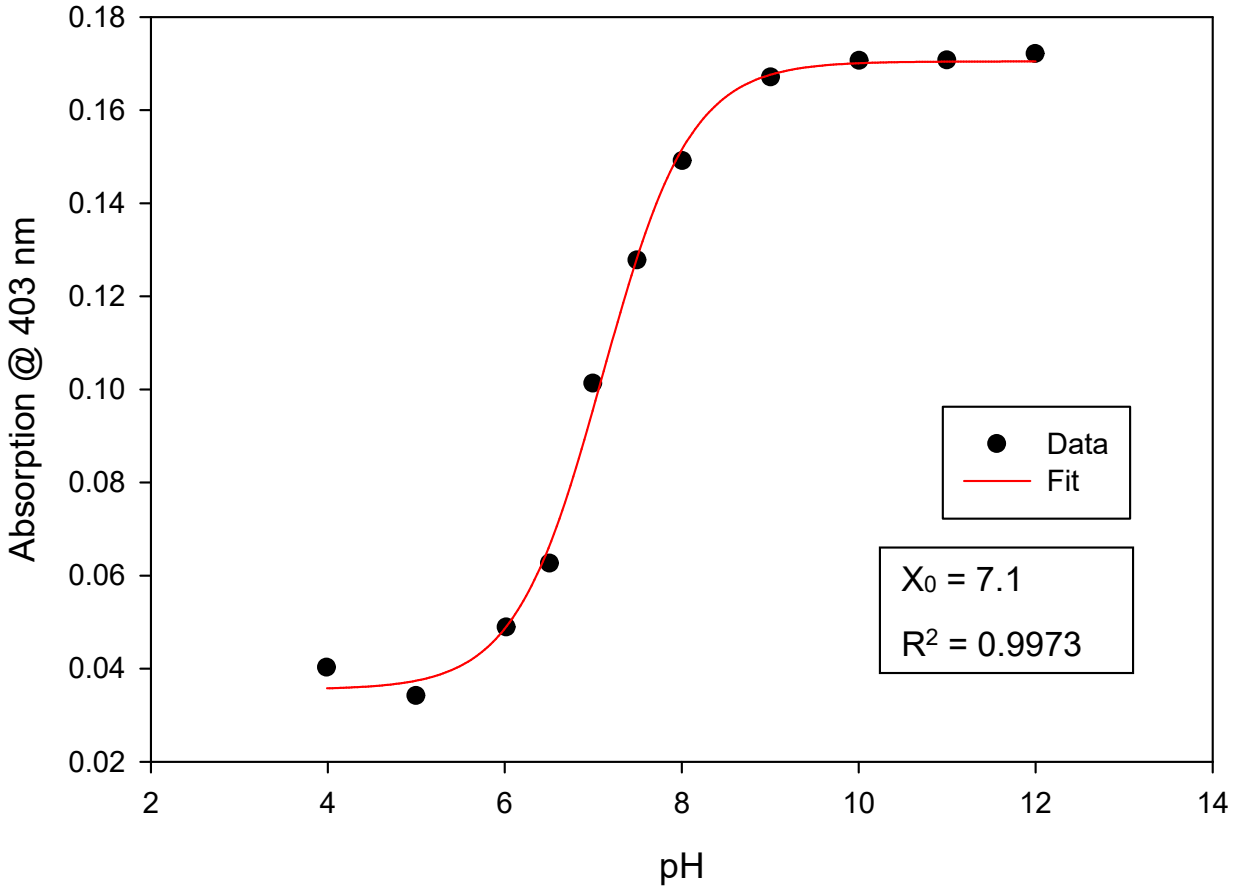


Figure S87. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***7****.*

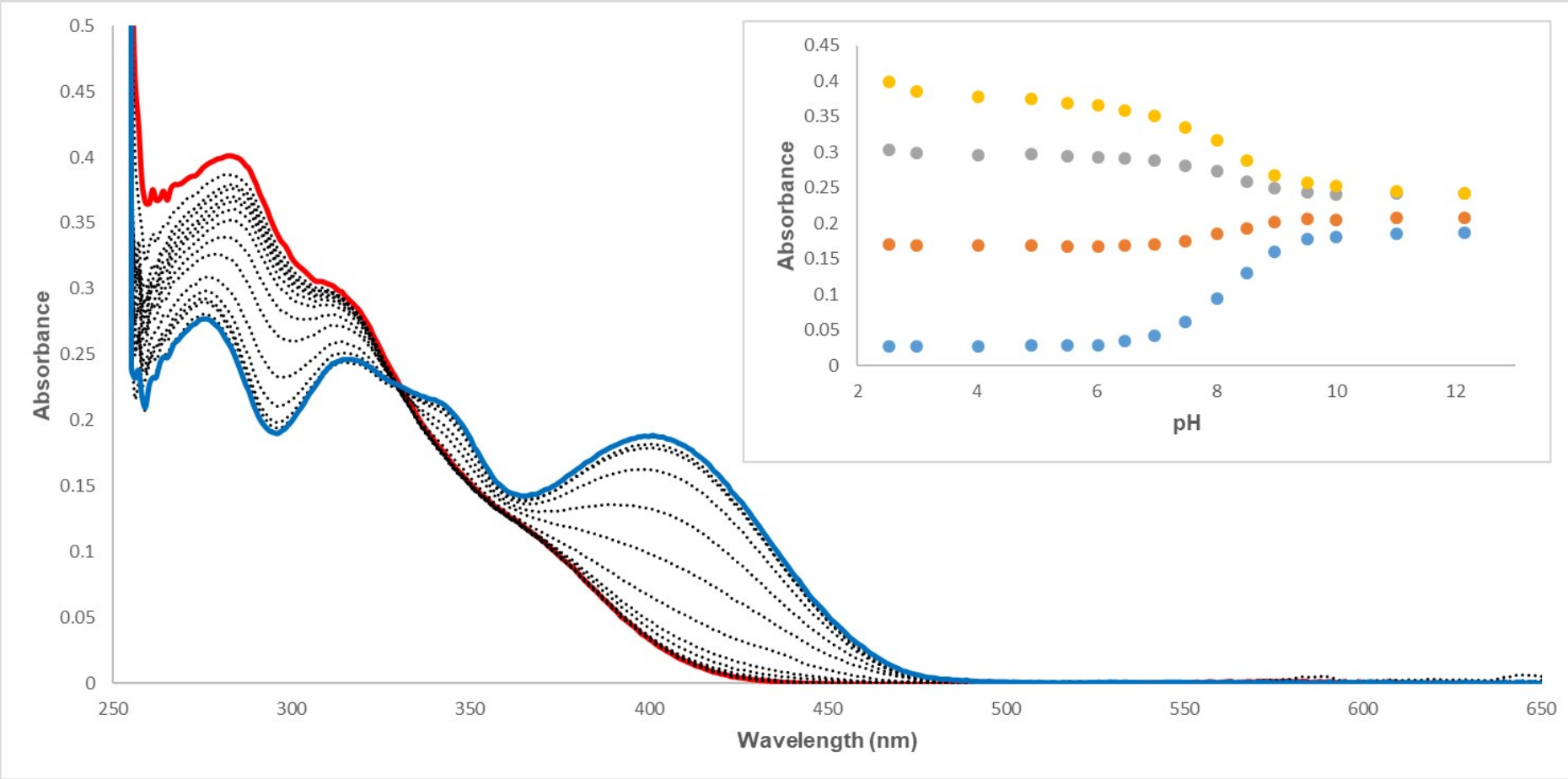


Figure S88. *Absorption spectra taken over the course of a pH-spectrophotometric titration of* ***8*** *(10 µM) in an DMSO–water mixture (9/1 v/v; in presence of 0.1 M TBAPF6) pH 2.53 (red), pH 12.14 (blue). Inset: Comparison plots of absorbance at 285 nm (yellow), 311 nm (grey), 344 nm (orange), and 404 nm (blue) vs. pH.*

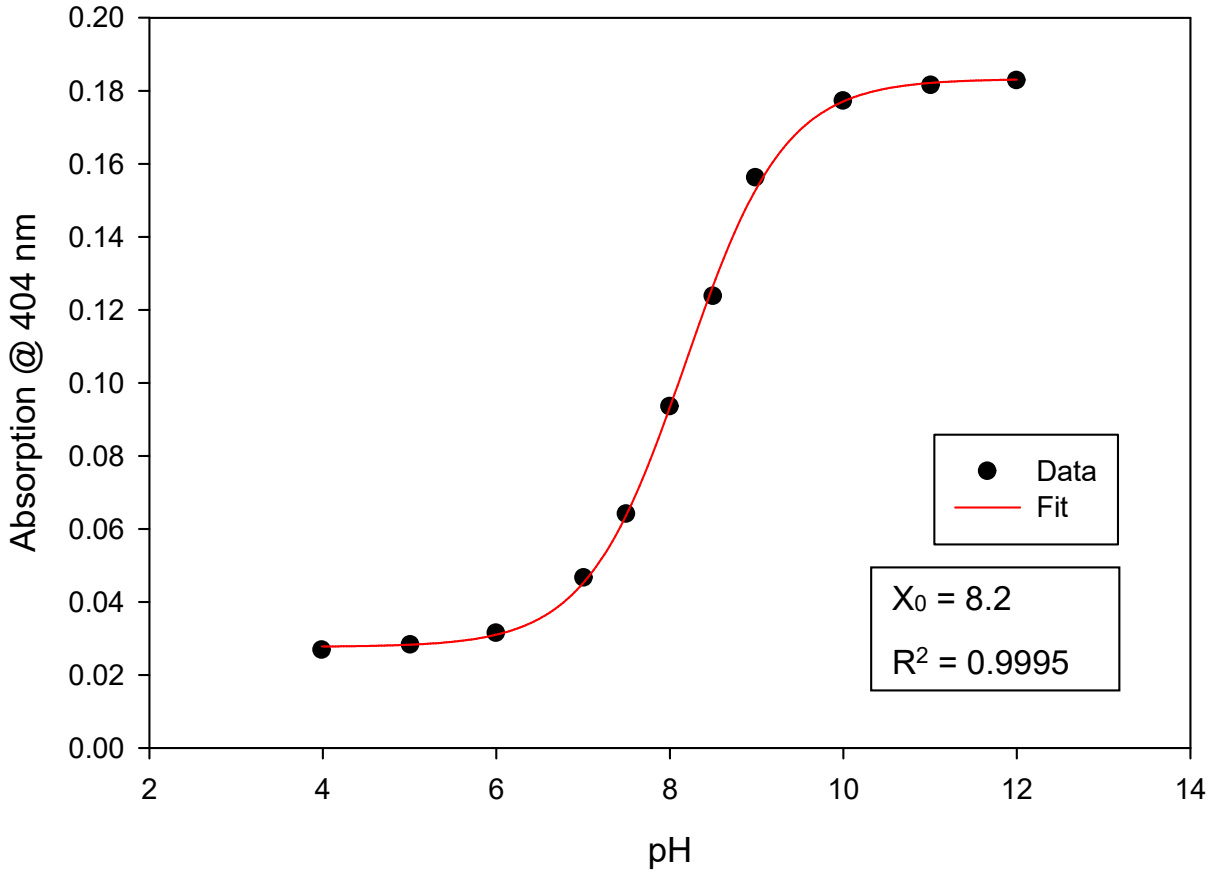


Figure S89. *Four parameter sigmoid curve fit with the point of inflexion (X_0) corresponding to the pK_a value for* ***8****.*

^{1}H NMR Anion Binding Screen:

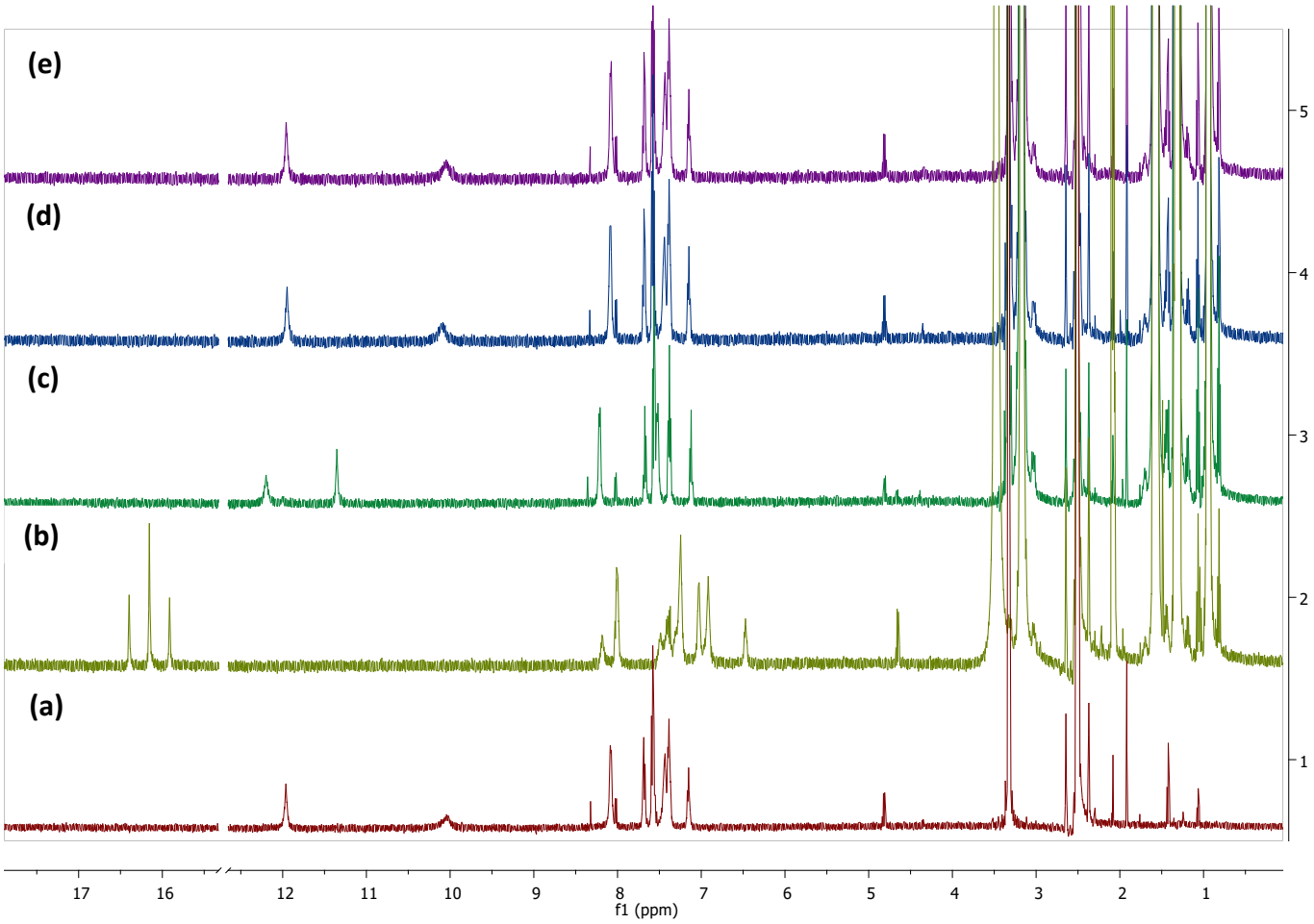


Figure S90. *^{1}H NMR stackplot of **1** (2.5 x 10^{-6} M) treated with different TBA salts of anions (10 equiv.). a) Blank spectra of **1** (no anion present). b) **1** + TBAF. c) **1** + TBACl. d) **1** + TBABr. e) **1** + TBAI.*

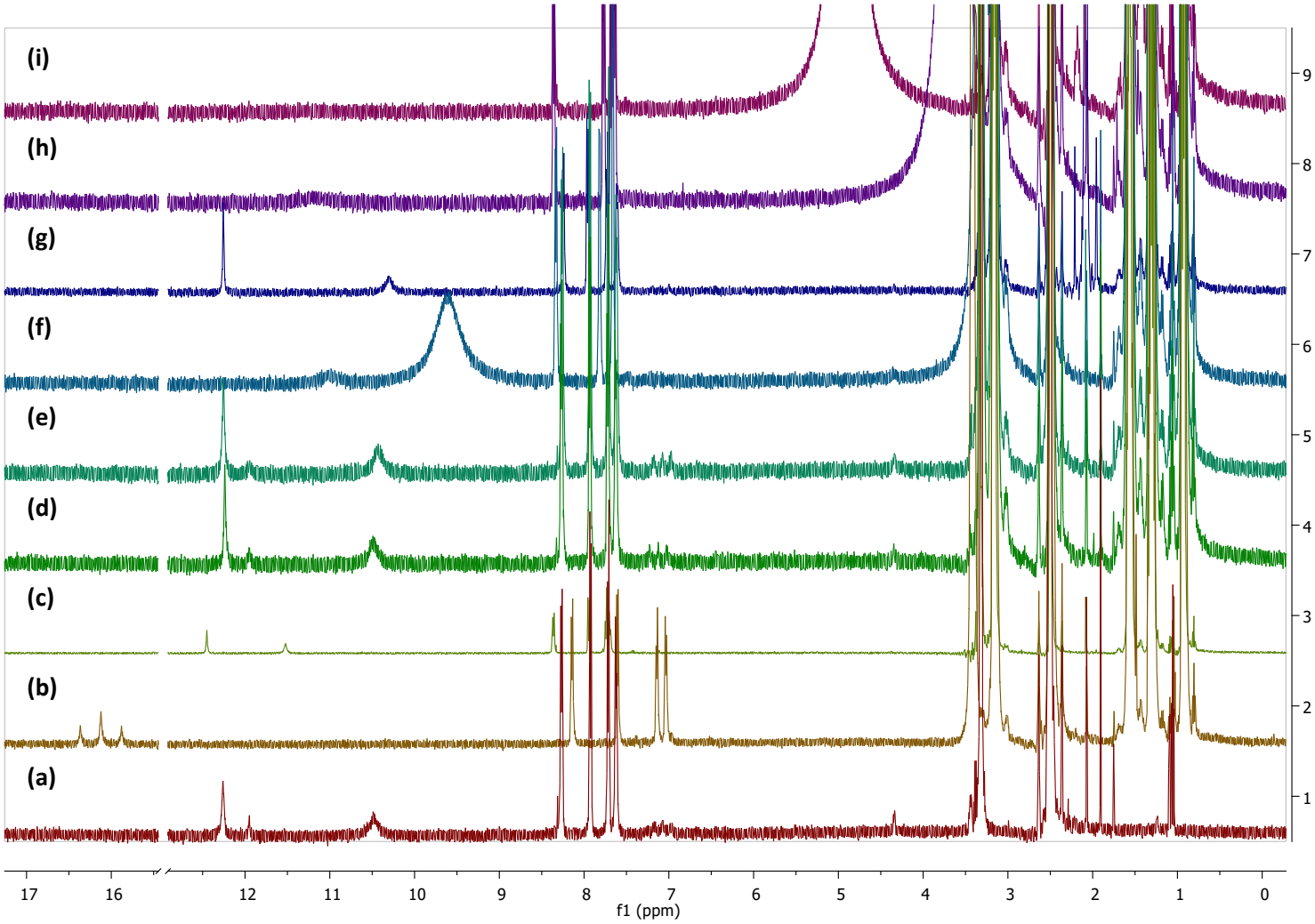


Figure S91. *^{1}H NMR stackplot of **2** (2.5 x 10^{-6} M) treated with different TBA salts of anions (10 equiv.). a) Blank spectra of **2** (no anion present). b) **2** + TBAF. c) **2** + TBACl. d) **2** + TBABr. e) **2** + TBAI, f) **2** + TBA_2SO_4, g) **2** + $TBANO_3$, h) **2** + TBAOAc, i) **2** + $TBA_2H_2PO_4$.*

^{1}H NMR Anion Binding and Fitting Data:

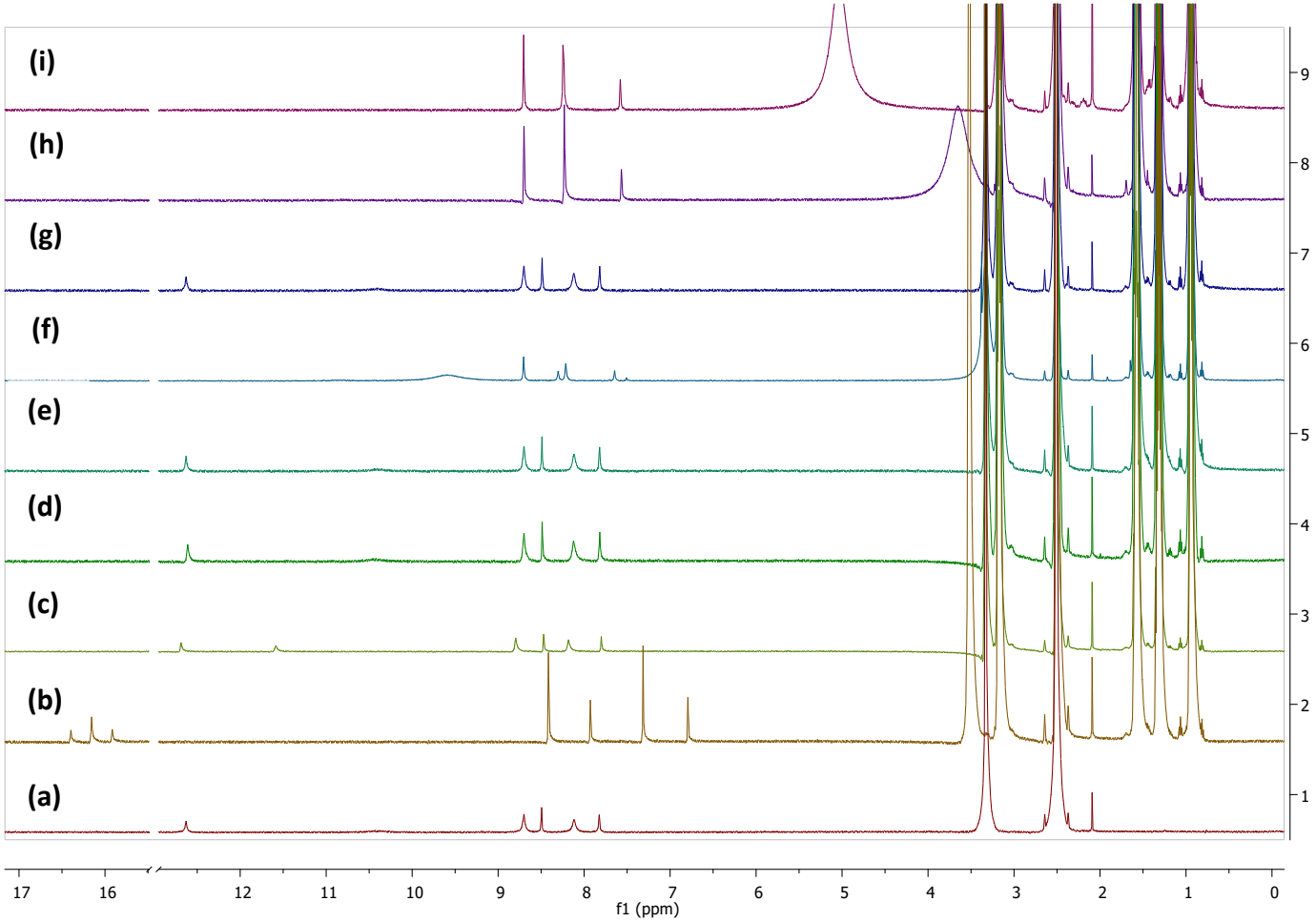


Figure S92. *^{1}H NMR stackplot of **3** (2.5 x 10^{-6} M) treated with different TBA salts of anions (10 equiv.). a) Blank spectra of **3** (no anion present). b) **3** + TBAF. c) **3** + TBACl. d) **3** + TBABr. e) **3** + TBAI, f) **3** + TBA_2SO_4, g) **3** + $TBANO_3$, h) **3** + TBAOAc, i) **3** + $TBA_2H_2PO_4$.*

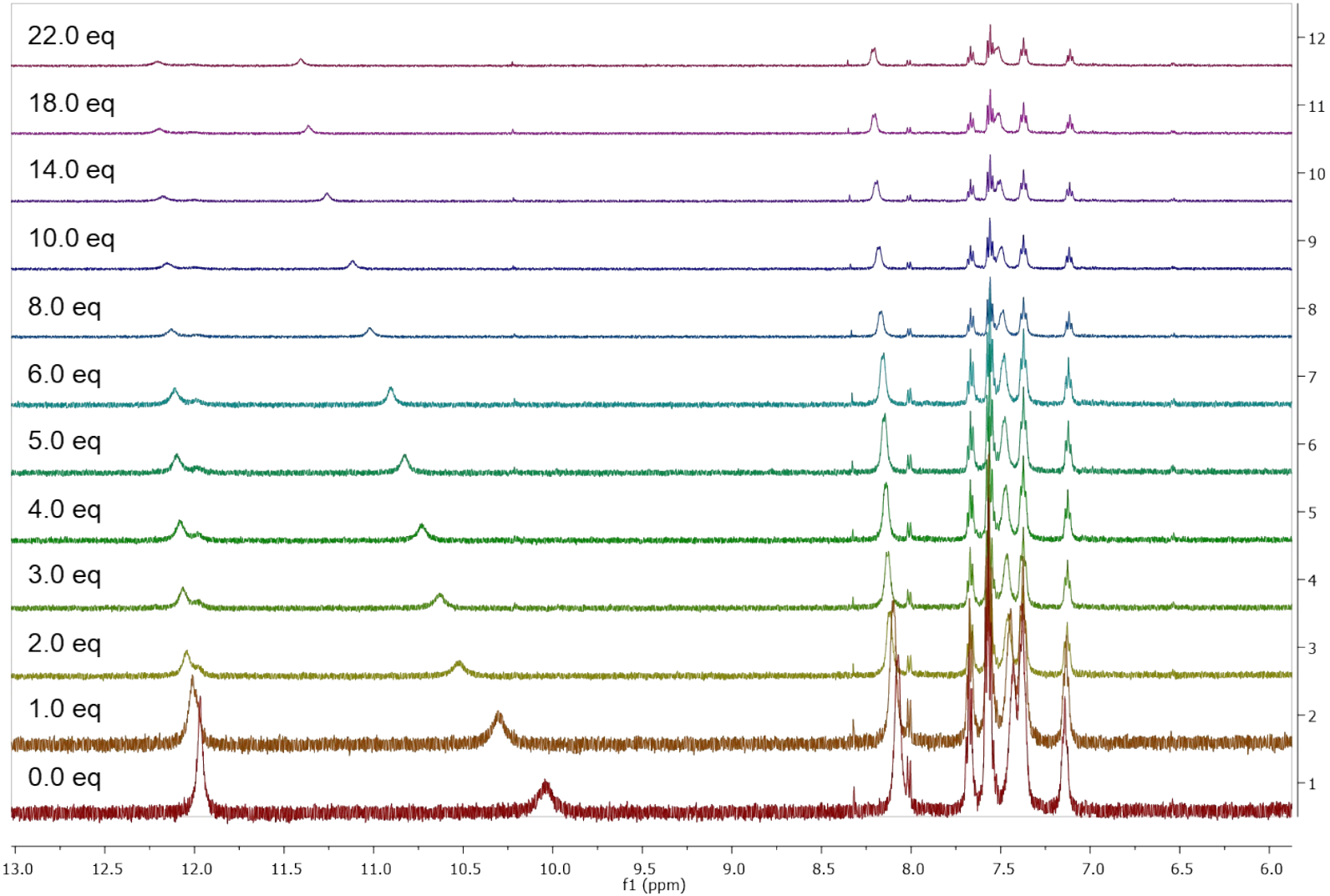


Figure S93. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **1** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

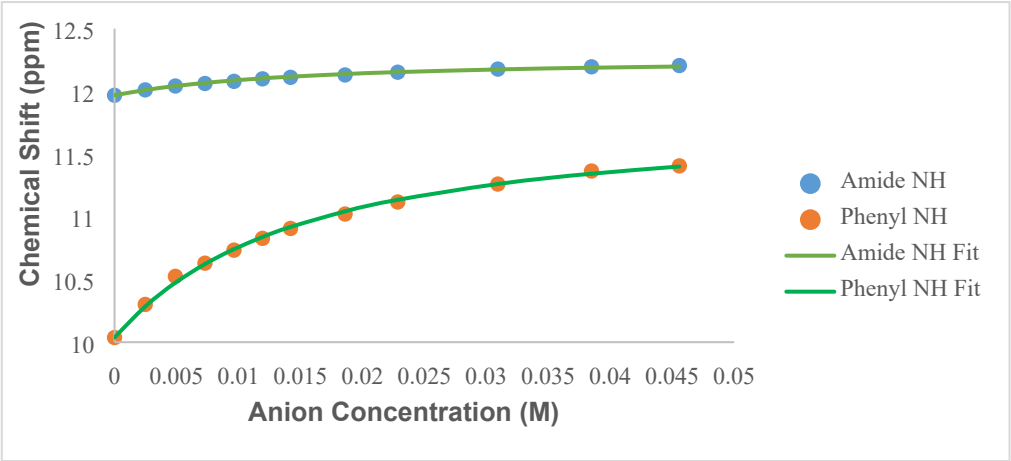


Figure S94. *Fitted binding isotherm for the titration of* ***1*** *(2.5 X 10^{-6} M) in the presence of increasing concentrations of Cl^- in DMSO-d_6/0.5% H_2O). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration. Ka = 76 M^{-1}, Error = 2.63 %.*

http://app.supramolecular.org/bindfit/view/6d463652-057f-4ea4-b397-8bb063aa3489

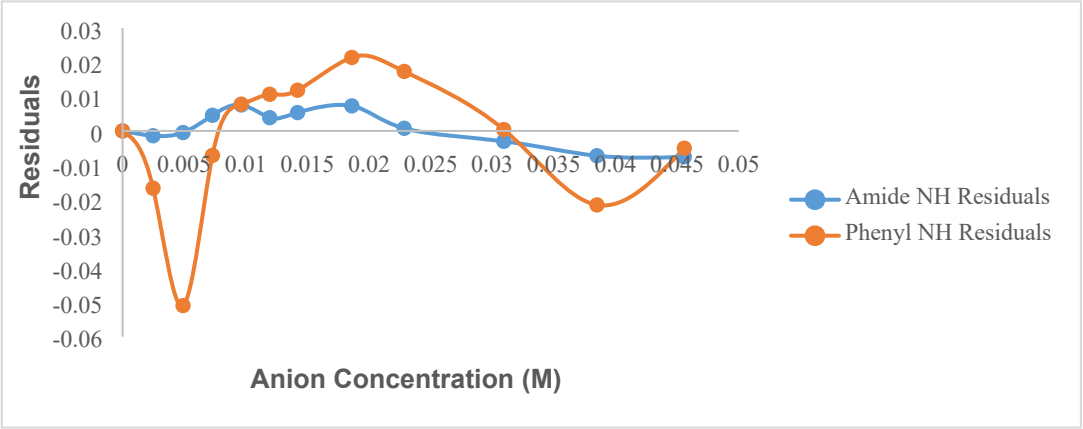


Figure S95. *Residual plot of* ***1.***

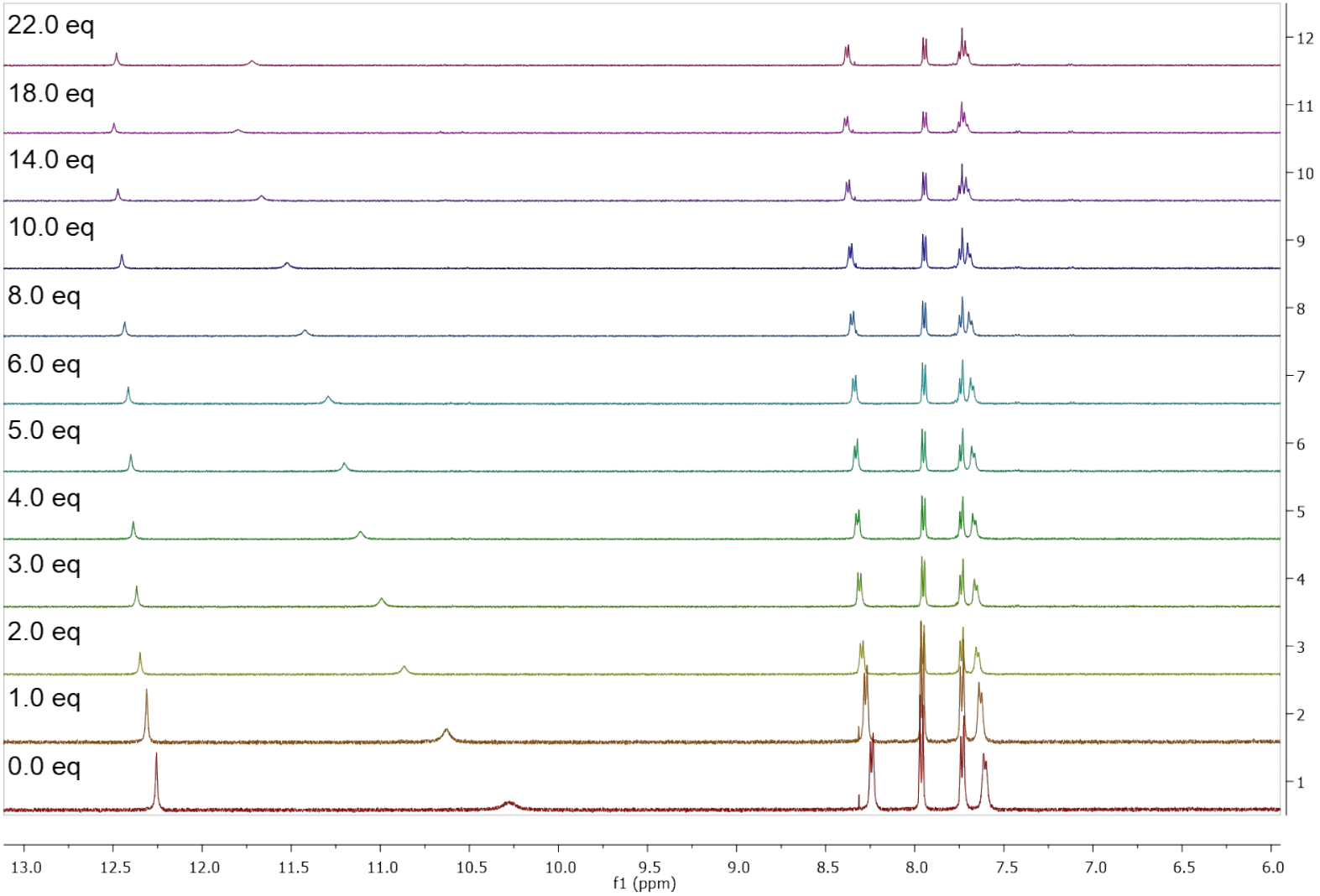


Figure S96. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **2** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

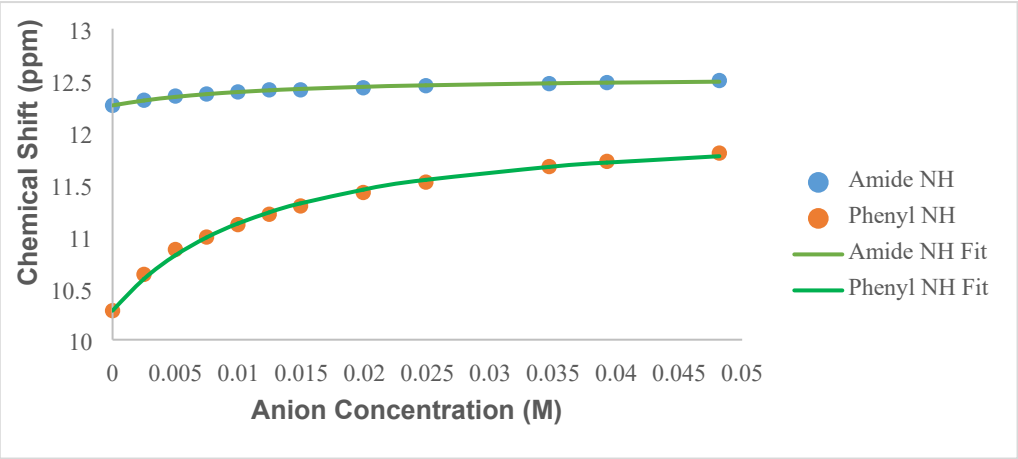


Figure S97. *Fitted binding isotherm for the titration of* ***2*** *(2.5 X 10^{-6} M) in the presence of increasing concentrations of Cl^- in DMSO-d_6/0.5% H_2O). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration. Ka = 97 M^{-1}, Error = 3.58 %.*

http://app.supramolecular.org/bindfit/view/b9c881e2-2f89-47fd-bf93-a6d2d3a9006d

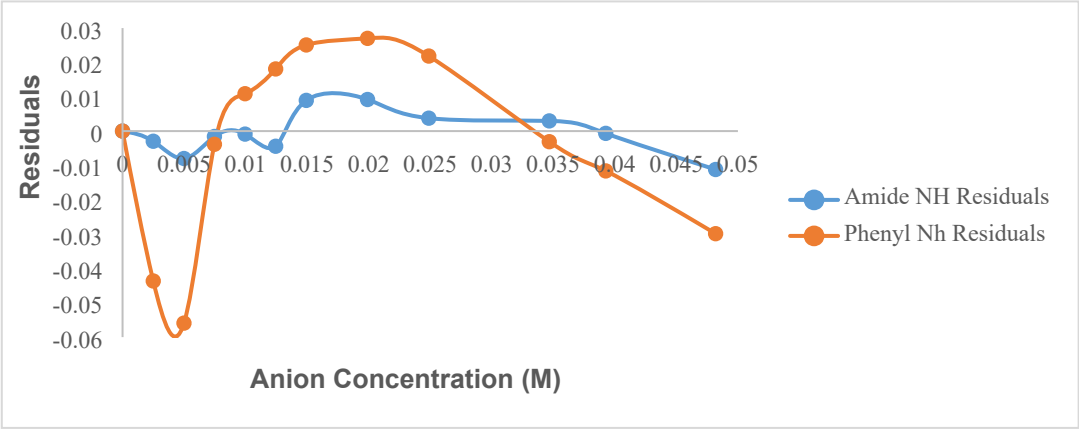


Figure S98. *Residual plot of* ***2***

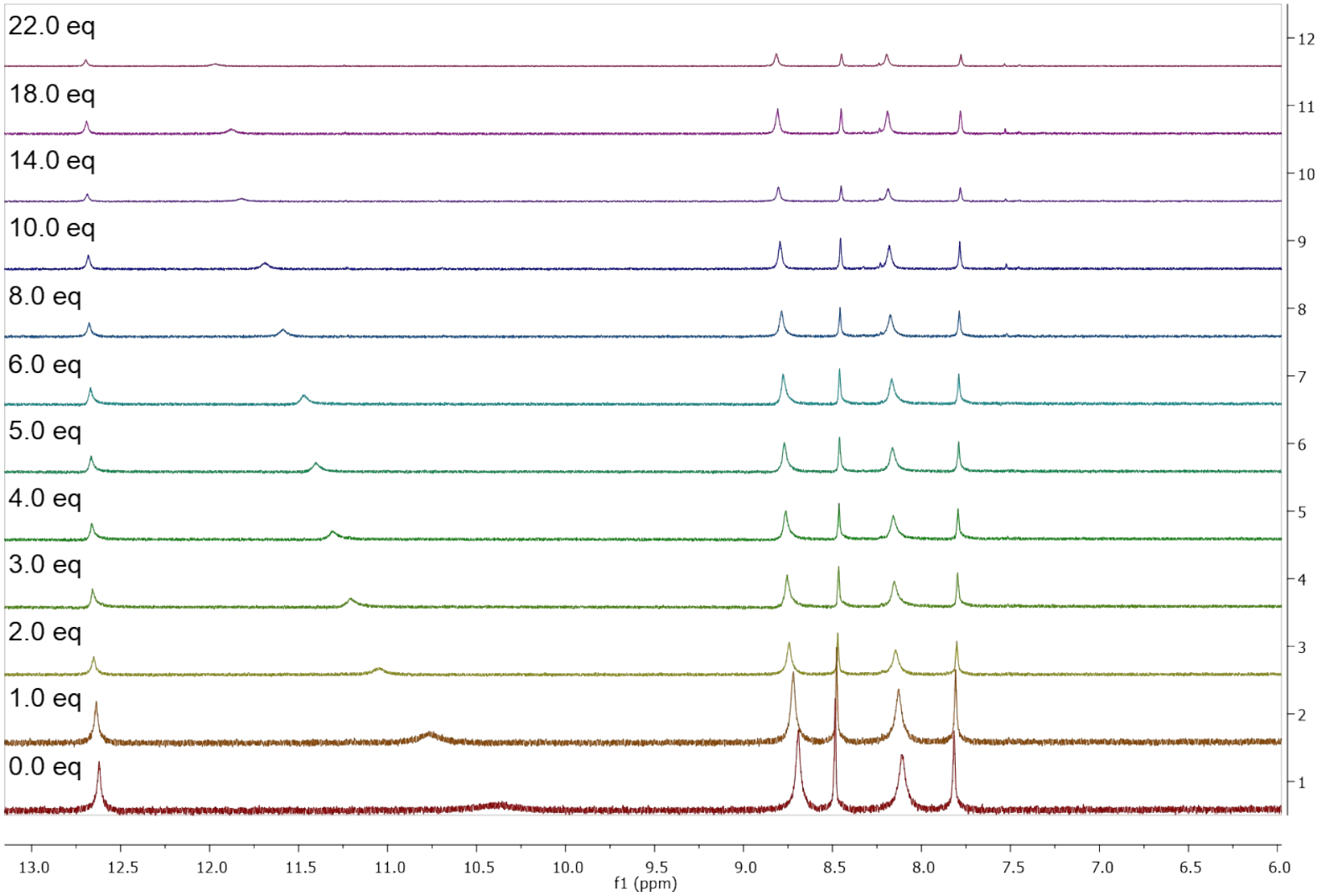


Figure S99. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **3** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

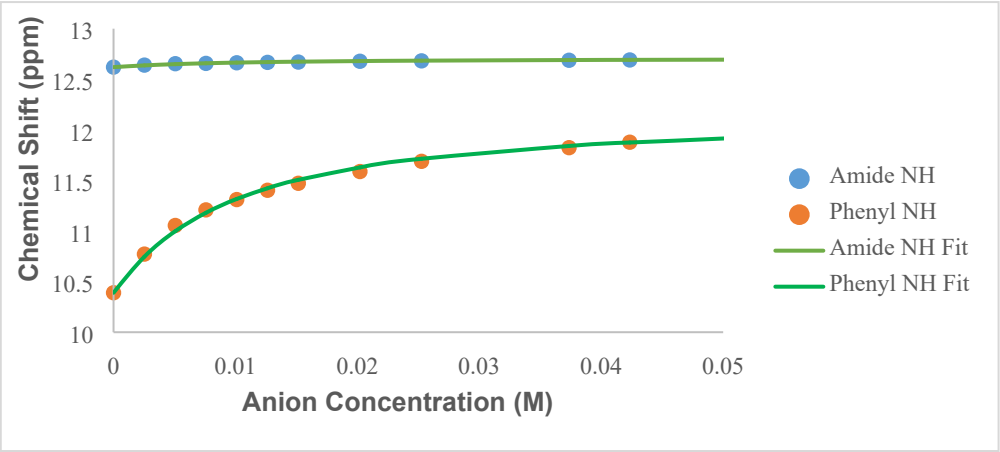


Figure S100. *Fitted binding isotherm for the titration of* ***3*** *(2.5 X 10^{-6} M) in the presence of increasing concentrations of Cl^- in DMSO-d_6/0.5% H_2O). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration. K_a = 123 M^{-1}, Error = 4.78 %.* http://app.supramolecular.org/bindfit/view/7ab90122-e3d8-4bfe-9e82-db25ca1e360d

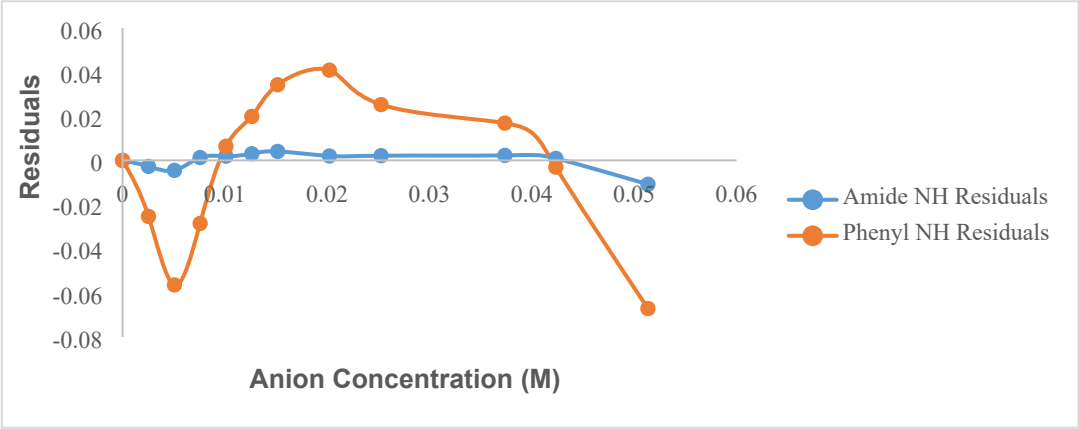


Figure S101. *Residual plot of* ***3.***

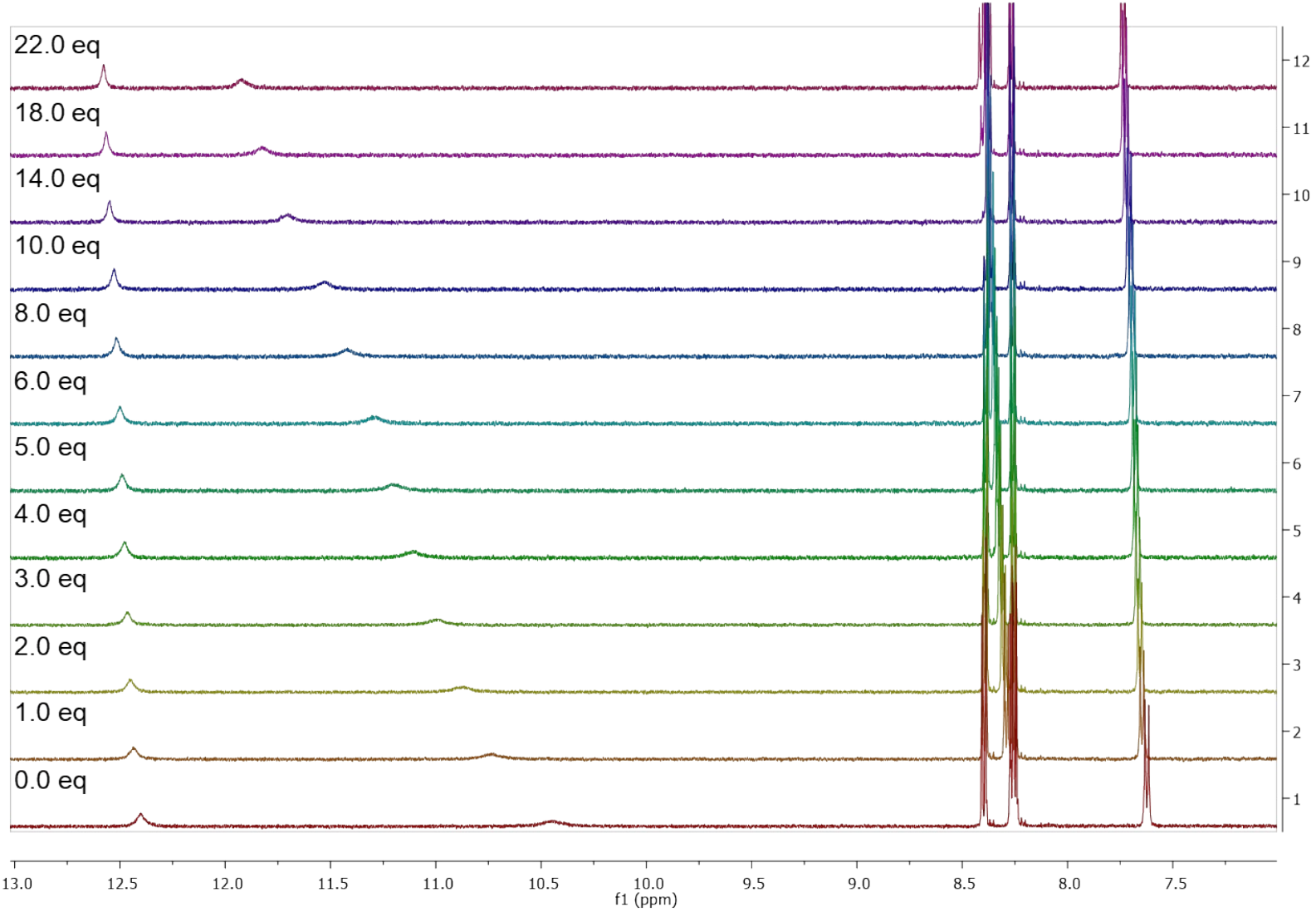


Figure S102. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **4** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

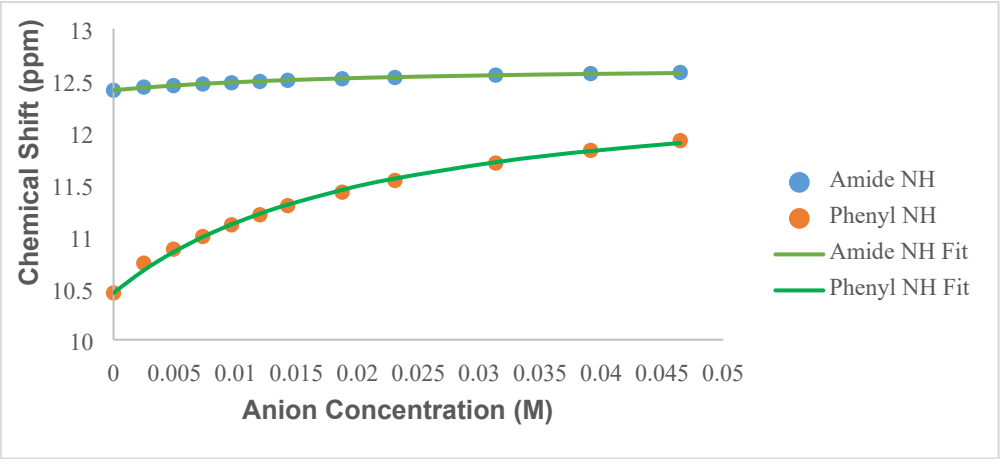


Figure S103. *Fitted binding isotherm for the titration of* ***4*** *(2.5 X* 10^{-6} *M) in the presence of increasing concentrations of* Cl^- *in DMSO-*d_6*/0.5%* H_2O*). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration.* K_a *= 54* M^{-1}*, Error = 2.85 %.*

http://app.supramolecular.org/bindfit/view/6b4ba0e4-dbef-48ed-9366-bac9f2b33226

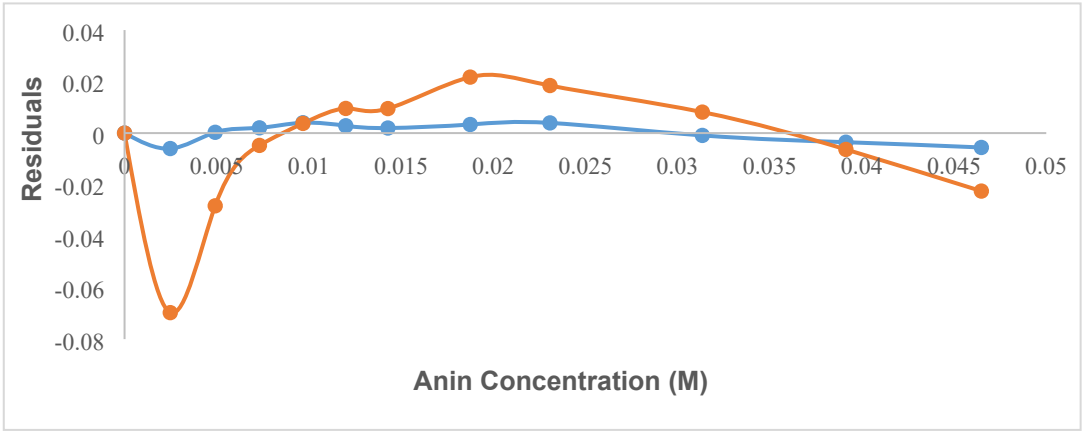


Figure S104. *Residual plot of* ***4.***

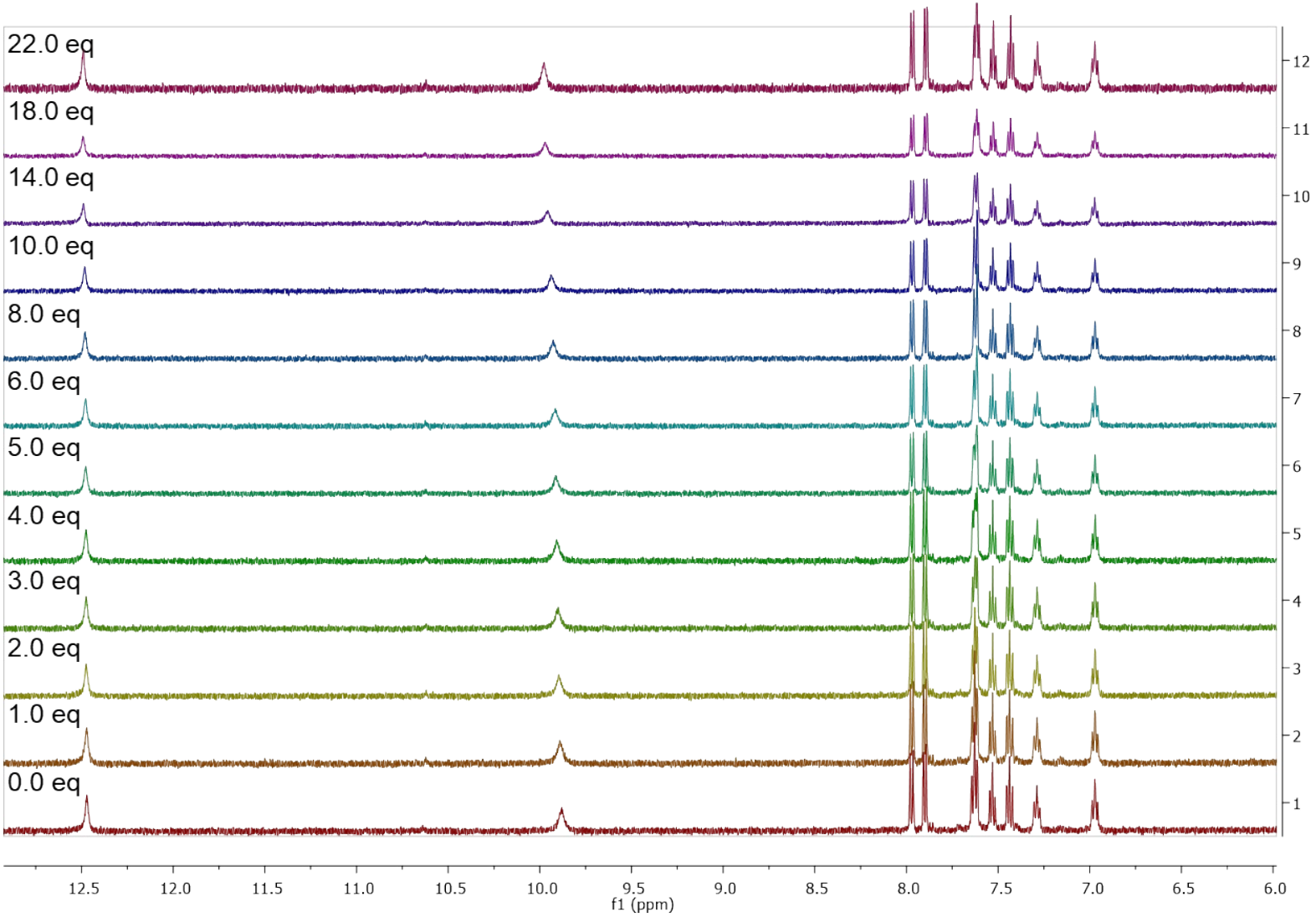


Figure S105. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **5** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

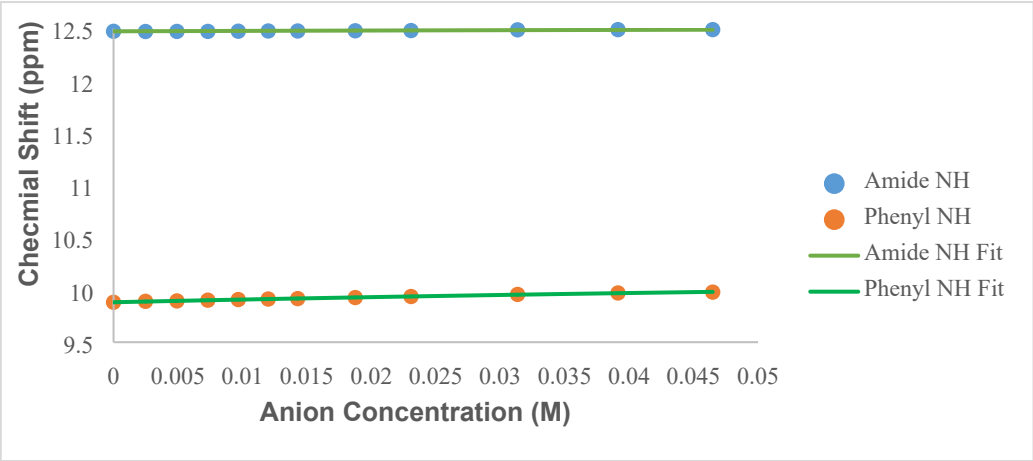


Figure S106. *Fitted binding isotherm for the titration of* ***5*** *(2.5 X 10^{-6} M) in the presence of increasing concentrations of Cl^- in DMSO-d_6/0.5% H_2O). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration. K_a = 6, Error = 3.19 %.*

http://app.supramolecular.org/bindfit/view/808f07cd-6477-471e-b172-c6dab49a4405

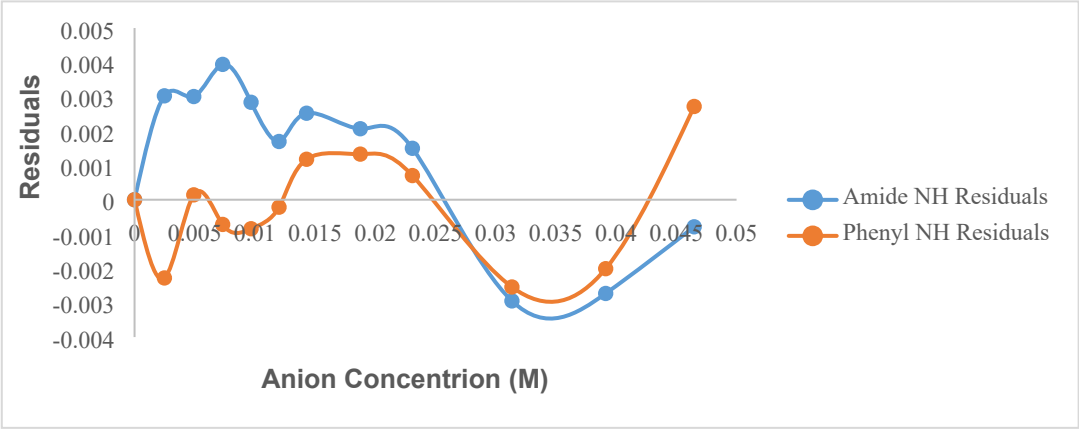


Figure S107. *Residual plot of* ***5.***

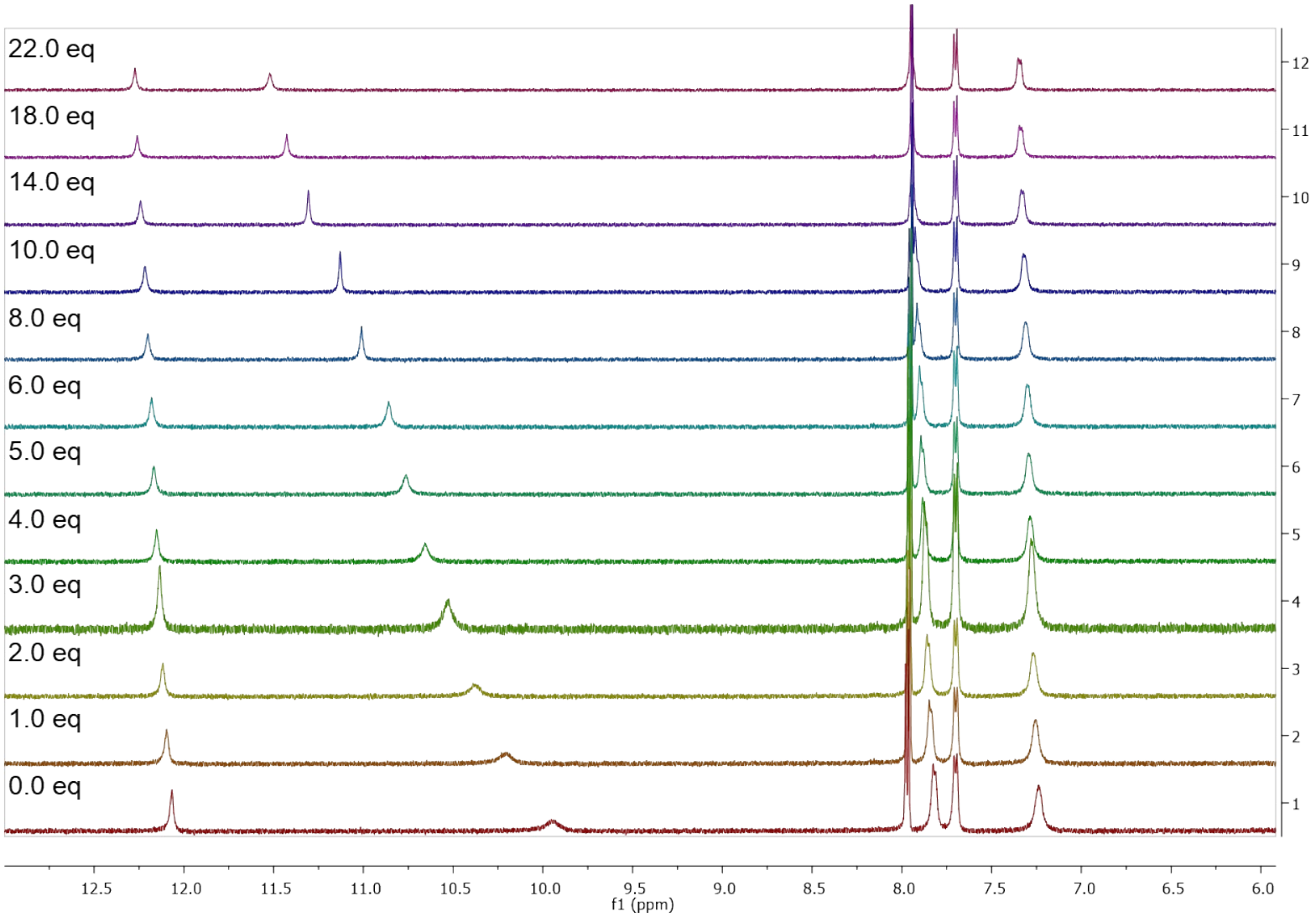


Figure S108. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **6** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

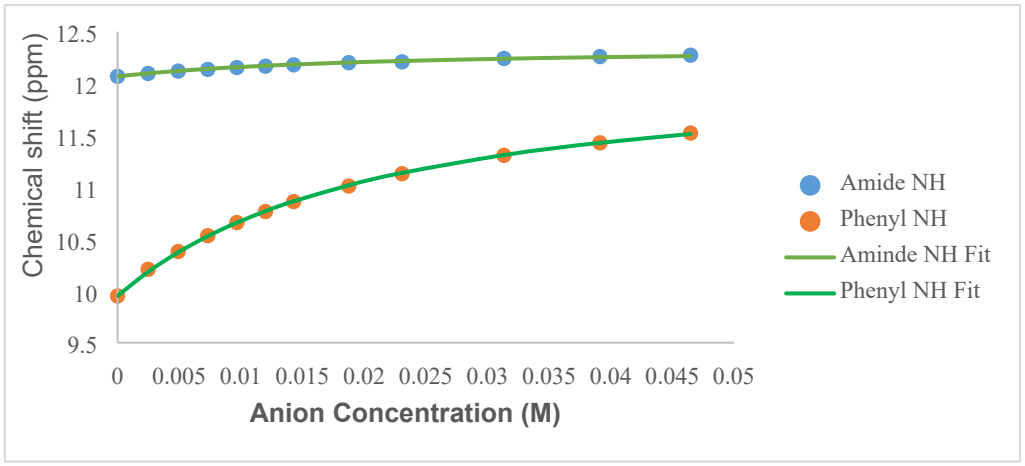


Figure S109. *Fitted binding isotherm for the titration of* ***6*** *(2.5 X* 10^{-6} *M) in the presence of increasing concentrations of* Cl^- *in DMSO-*d_6*/0.5%* H_2O*). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration.* K_a *= 52* M^{-1}*, Error = 1.85 %.*

http://app.supramolecular.org/bindfit/view/6f078276-c677-4a18-8a3d-1b13a398beff

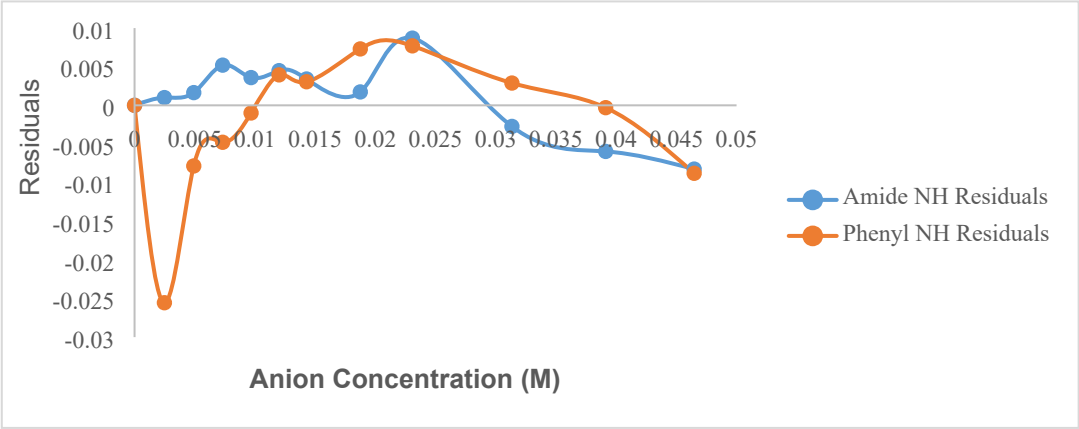


Figure S110. *Residual plot of* ***6.***

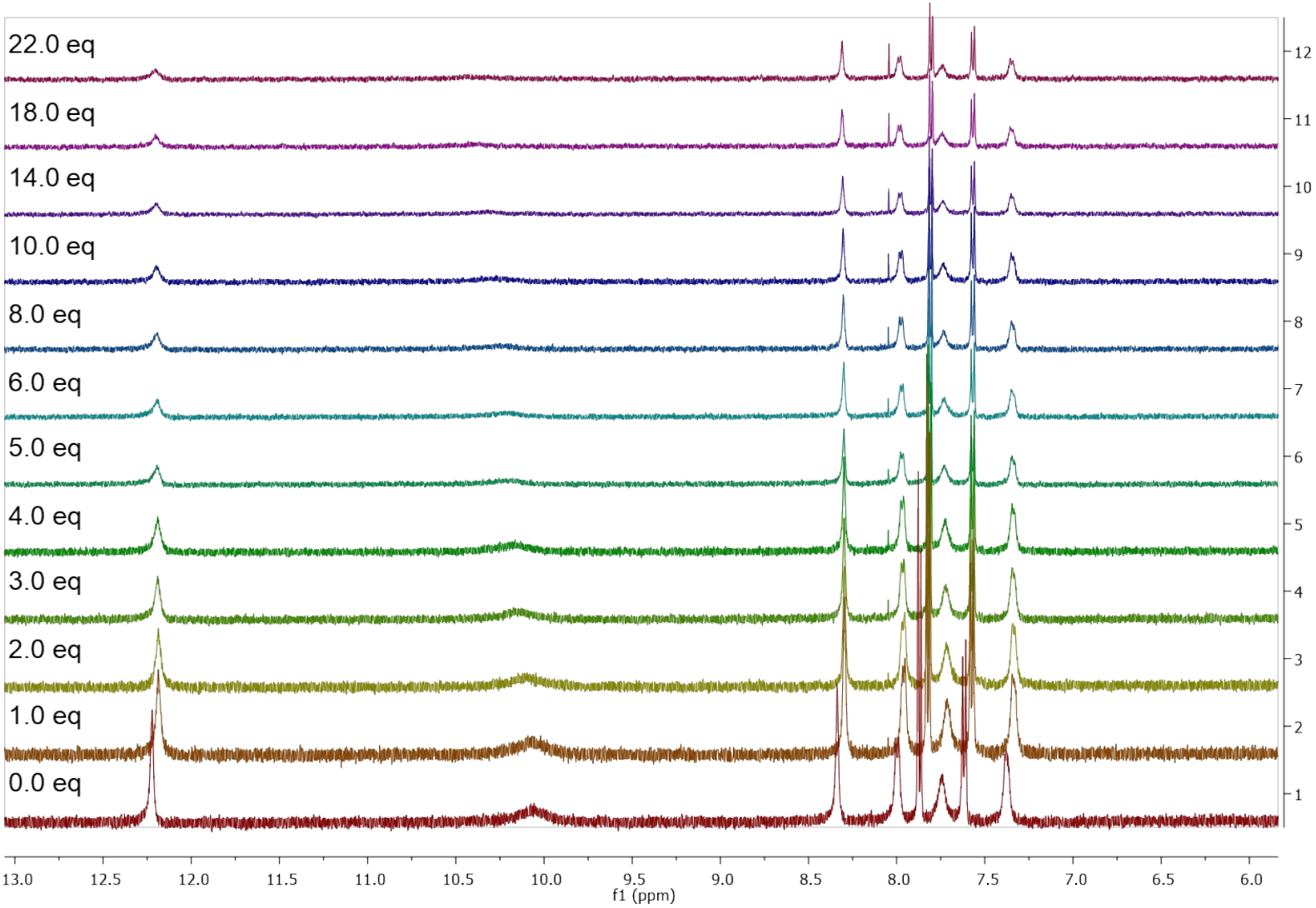


Figure S111. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **7** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

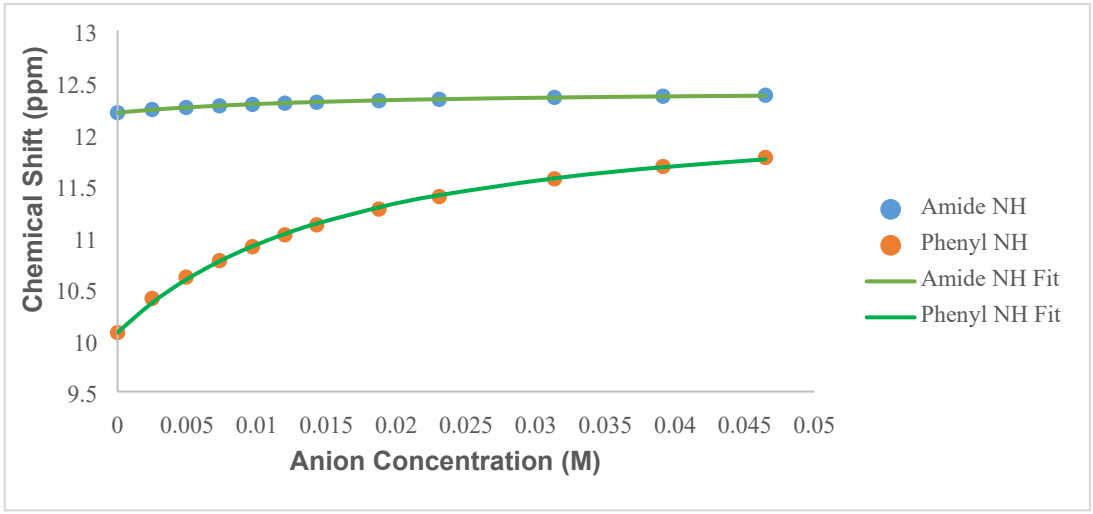


Figure S112. *Fitted binding isotherm for the titration of* ***7*** *(2.5 X 10^{-6} M) in the presence of increasing concentrations of Cl^- in DMSO-d_6/0.5% H_2O). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration. K_a = 69 M^{-1}, Error = 1.06 %.* http://app.supramolecular.org/bindfit/view/b58c6396-d702-49ec-aa8e-9772fcc0b312

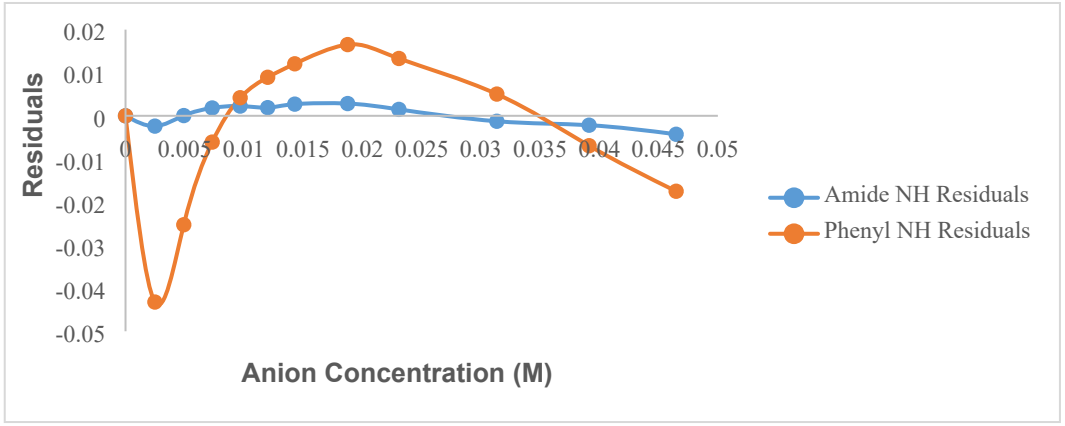


Figure S113. *Residual plot of* ***7.***

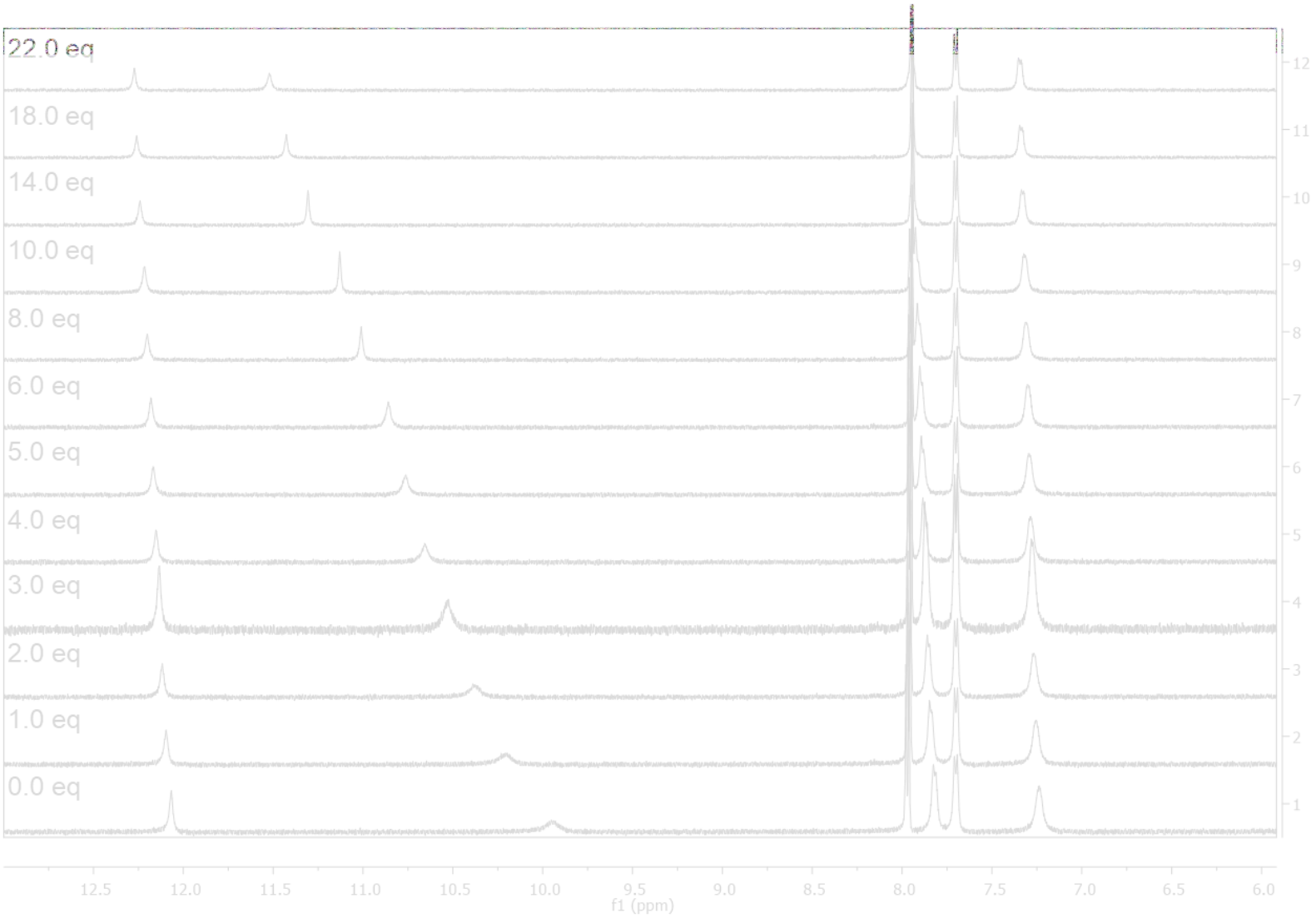


Figure S114. *^{1}H NMR stackplot, 6.0 ppm – 13.0 ppm, of receptor **8** with 0.0 – 22.0 equiv. TBACl in DMSO-d_6/0.5% H_2O.*

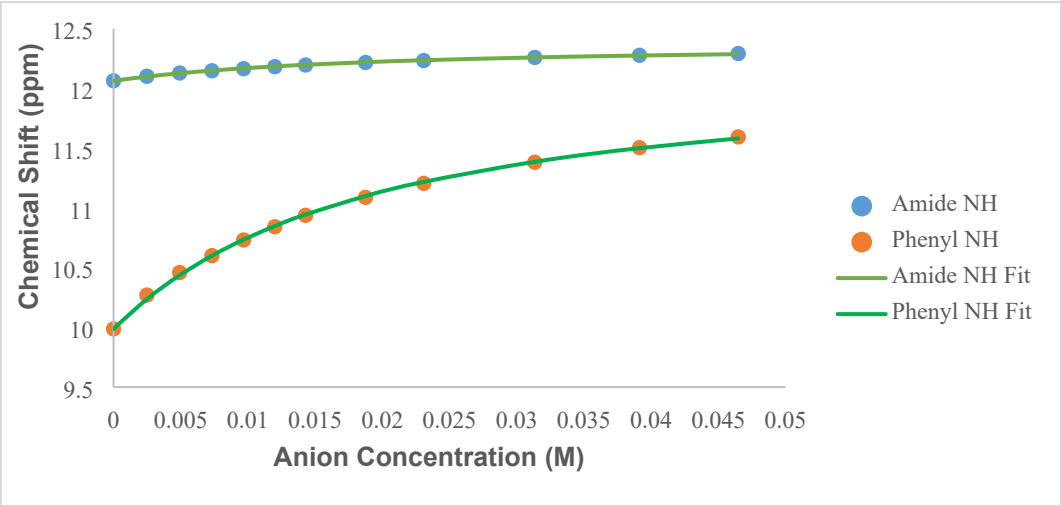


Figure S115. *Fitted binding isotherm for the titration of* ***8*** *(2.5 X 10^{-6} M) in the presence of increasing concentrations of Cl^- in DMSO-d_6/0.5% H_2O). The data is fitted to a 1:1 binding model and shows the chemical shift of the NH signals throughout the titration. K_a = 58 M^{-1}, Error = 1.47 %.* http://app.supramolecular.org/bindfit/view/400a20c4-bf6c-4161-aa3d-d9e742573a34

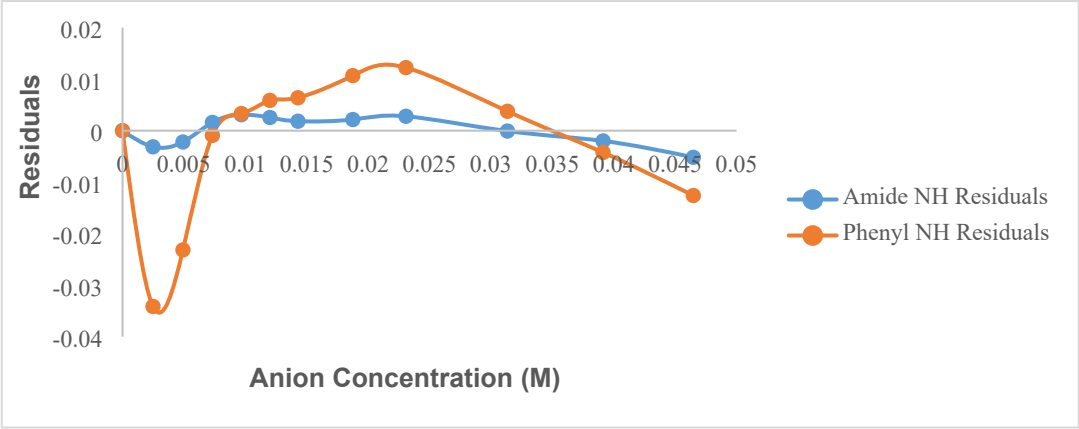


Figure S116. *Residual plot of* ***8.***

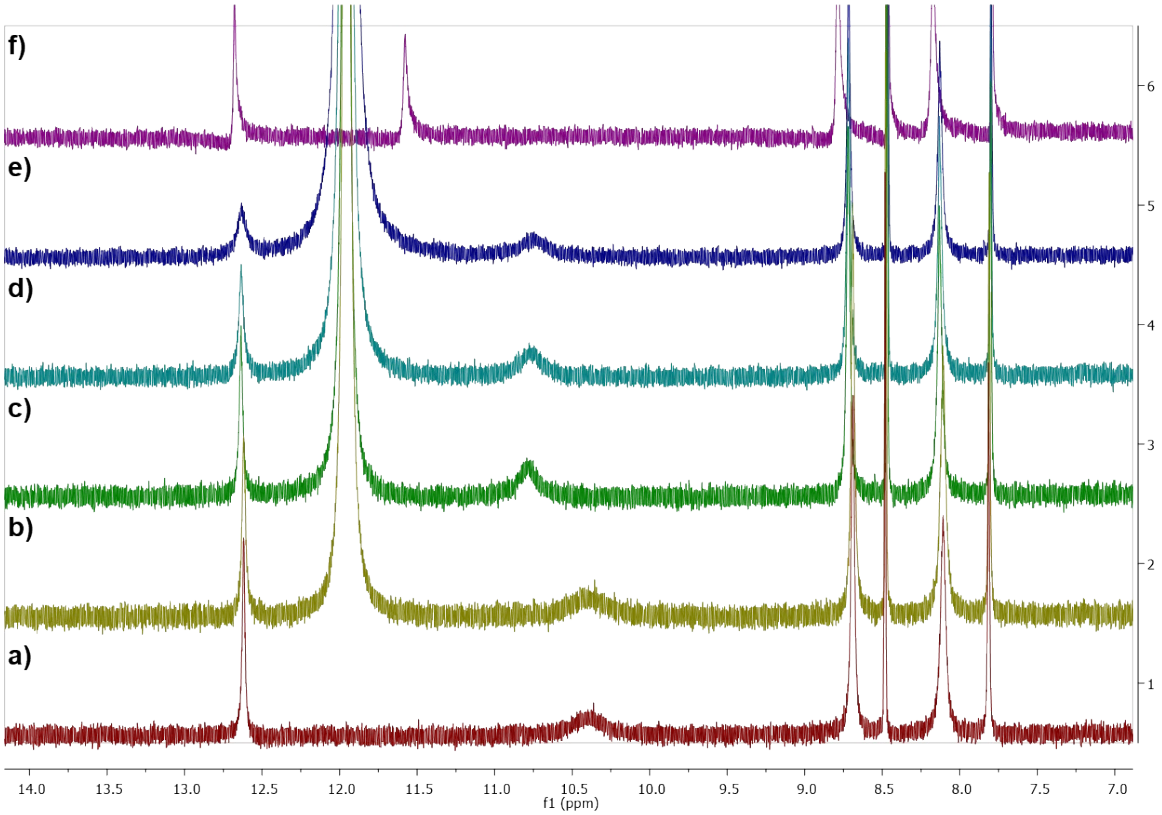


Figure S117. *^{1}H NMR stackplot of **3** (2.5 x 10^{-6} M) and TBACl (10 equiv.), treated with increasing additions of AcOH. a) **3** (no AcOH or TBACl). b) **3** + 10 equiv. AcOH. c) **3** + 10 equiv. AcOH + TBACl. d) **3** + 20 equiv. AcOH + 10 equiv. TBACl e) **3** + 100 equiv AcOH + 10 equiv. TBACl. f) **3** + 10 equiv. TBACl.*

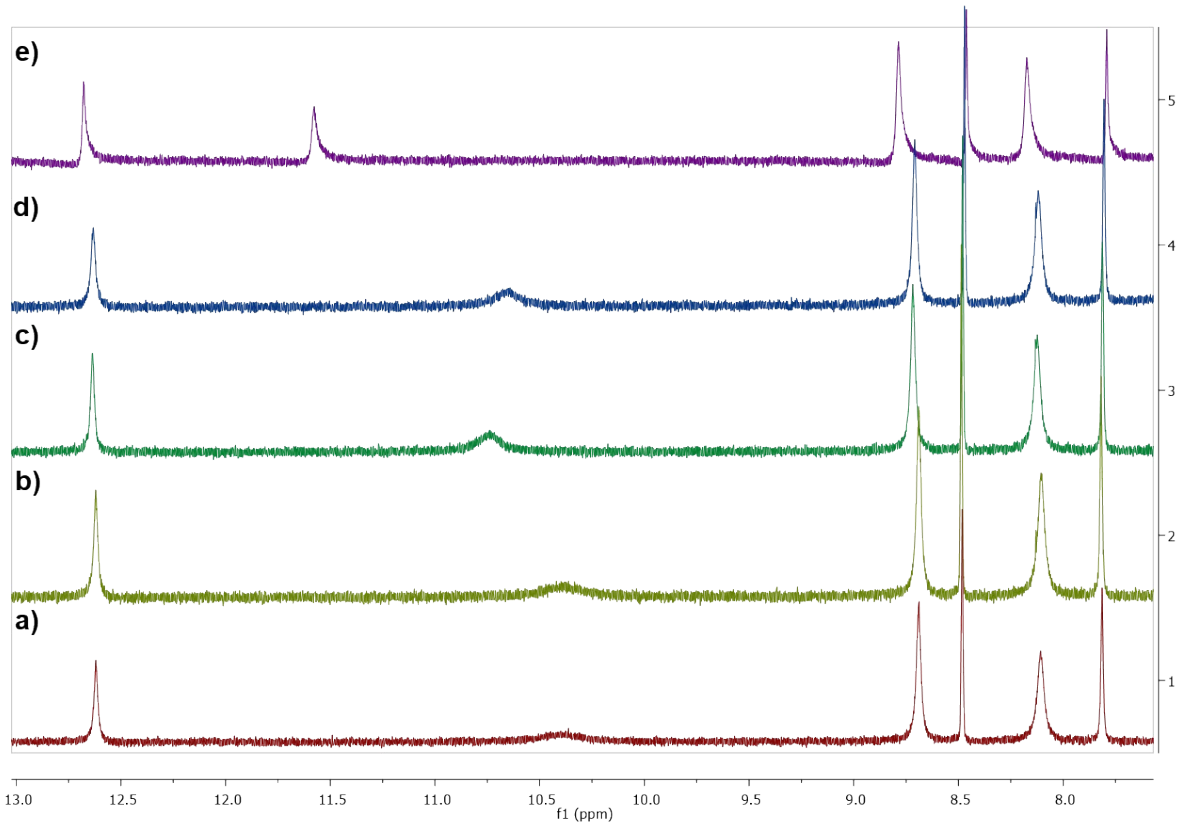


Figure S118. *^{1}H NMR stackplot of **3** (2.5 x 10^{-6} M) and TBACl (10 equiv.), treated with increasing additions of TFA. a) **3** (no AcOH or TBACl). b) **3** + 10 equiv. TFA. c) **3** + 10 equiv. TFA + TBACl. d) **3** + 20 equiv. TFA + 10 equiv. TBACl e) **3** + 100 equiv TFA + 10 equiv. TBACl. f) **3** + 10 equiv. TBACl.*

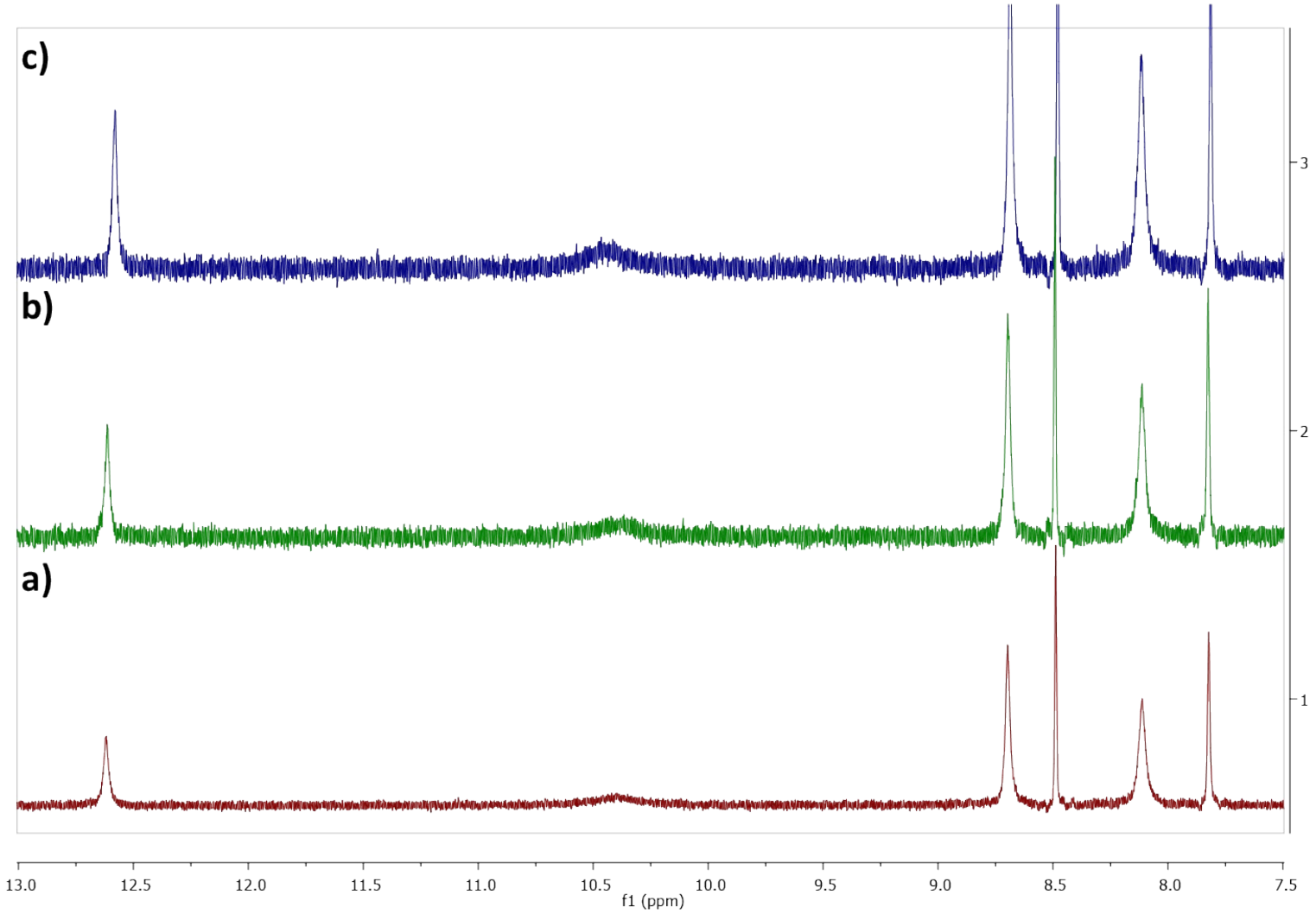


Figure S119. *^{1}H NMR stackplot of **3** (2.5 x 10^{-6} M) treated with increasing additions of CSA. a) **3** (no CSA). b) **3** + 10 equiv. CSA. c) **3** + 100 equiv. CSA.*

Geometry Optimisations:

34
SCF Energy = -989.818171042
Enthalpy 0K = -989.557856
Enthalpy 298K = -989.538977
Free Energy 298K = -989.606784
Lowest Frequencies = 22.0973 cm-1
ASQ1_a
C 5.48112 -1.98683 0.12866
C 4.34430 -2.79366 0.10147
C 3.07856 -2.22042 0.05940
C 2.93895 -0.82746 0.04472
C 4.07143 -0.01072 0.07323
C 5.33261 -0.60121 0.11393
N 1.62139 -0.32816 0.00629
C 1.16539 0.92720 -0.04602
C 1.74145 2.33746 -0.09652
O 2.83291 2.83548 -0.10453
C -0.12745 1.44505 -0.07851
N -1.42786 1.00272 -0.06037
C -3.31356 -0.53754 0.01364
C -4.21075 0.40741 0.52310
C -5.57334 0.12320 0.55823
C -6.04371 -1.10017 0.08286
C -5.14927 -2.04763 -0.41599
C -3.78661 -1.77106 -0.44393
C 0.29278 2.83828 -0.12715
O -0.29213 3.89492 -0.17179
H -2.12113 1.74012 -0.13370
H 0.87373 -1.02278 -0.00461
H 3.97649 1.06881 0.06067
H 2.19254 -2.85036 0.03777
H 4.43906 -3.87522 0.11253
H 6.46987 -2.43291 0.16095
H 6.20892 0.03962 0.13470
H -3.86054 1.35184 0.93124
H -6.26531 0.85425 0.96393
H -7.10713 -1.31771 0.10815
H -5.51449 -3.00237 -0.78100
H -3.07242 -2.49723 -0.81862
C -1.84061 -0.30909 -0.04952
O -1.03854 -1.23226 -0.10406

34
SCF Energy = -989.812210970
Enthalpy 0K = -989.552579
Enthalpy 298K = -989.533866
Free Energy 298K = -989.598732
Lowest Frequencies = 43.6932 cm-1
ASQ1_b
C 3.00349 -1.73728 -1.36391
C 1.83822 -1.41756 -2.05900
C 0.61421 -1.36804 -1.39726
C 0.56361 -1.61417 -0.02246
C 1.72530 -1.94063 0.67930
C 2.93887 -2.00935 0.00314
N -0.66549 -1.54662 0.67100
C -1.72632 -0.80917 0.30947
C -3.15043 -0.99382 0.71227
O -3.70293 -1.75548 1.45937
C -2.01932 0.32503 -0.43378
N -1.38296 1.26113 -1.19670
C 0.76479 1.53051 0.03784
C 0.20740 1.50574 1.31923
C 1.03640 1.39117 2.43341
C 2.41792 1.30387 2.27004
C 2.97586 1.35361 0.99113
C 2.15338 1.47705 -0.12158
C -3.47823 0.20724 -0.20183
O -4.44199 0.80242 -0.60600
H -1.95238 1.69894 -1.91816
H -0.83952 -2.23679 1.39465
H 1.67565 -2.11196 1.75135
H -0.29801 -1.15183 -1.94612
H 1.87485 -1.21172 -3.12436
H 3.95500 -1.78007 -1.88432
H 3.84203 -2.25736 0.55268
H -0.86565 1.60048 1.45627
H 0.60189 1.38091 3.42833
H 3.06132 1.20997 3.14007
H 4.05246 1.29351 0.86296
H 2.56676 1.52413 -1.12424
C -0.05360 1.70642 -1.19908
O 0.36934 2.27511 -2.18473

34
SCF Energy = -989.797109358
Enthalpy 0K = -989.538207
Enthalpy 298K = -989.518870
Free Energy 298K = -989.588397
Lowest Frequencies = 18.1971 cm-1
ASQ1_c
C -5.92830 -1.62963 -0.00684

C -4.99300 -2.47598 -0.60030
C -3.65240 -2.10999 -0.65650
C -3.23647 -0.89274 -0.10860
C -4.16326 -0.04401 0.49911
C -5.50440 -0.41766 0.53536
N -1.86009 -0.58173 -0.16460
C -1.26150 0.61561 0.00594
C -1.67575 2.06648 0.09708
O -2.70718 2.67741 0.10678
C 0.07672 0.94510 0.09090
N 1.20805 0.16761 0.13846
C 3.60437 -0.26178 -0.08517
C 3.67395 -1.06234 1.05915
C 4.80872 -1.83361 1.30116
C 5.87245 -1.80917 0.40063
C 5.80907 -1.00143 -0.73584
C 4.68109 -0.22374 -0.97549
C -0.16934 2.40093 0.22182
O 0.47787 3.39389 0.39249
H 1.14646 -0.77422 0.50584
H -1.25853 -1.34804 -0.44585
H -3.85085 0.90391 0.92078
H -2.92756 -2.76567 -1.13389
H -5.30522 -3.42316 -1.02929
H -6.97521 -1.91200 0.03281
H -6.22174 0.25094 1.00108
H 2.86932 -1.05630 1.79007
H 4.86641 -2.44328 2.19743
H 6.75549 -2.41215 0.58944
H 6.64146 -0.97548 -1.43212
H 4.61487 0.42290 -1.84500
C 2.42361 0.59835 -0.40218
O 2.48131 1.58434 -1.10048

33
SCF Energy = -989.276300545
Enthalpy 0K = -989.030920
Enthalpy 298K = -989.011992
Free Energy 298K = -989.080384
Lowest Frequencies = 18.8224 cm-1
ASQ1b_a
C 5.58842 -1.79169 0.05119
C 4.66589 -2.39992 0.90555
C 3.35055 -1.95196 0.95834
C 2.91396 -0.86679 0.17346
C 3.84898 -0.27595 -0.69986
C 5.16308 -0.73008 -0.75000
N 1.57200 -0.51192 0.25320
C 1.19674 0.70962 0.05775
C 1.80599 2.12559 -0.01406
O 2.91909 2.59631 -0.02851
C -0.08670 1.33523 0.01188
N -1.40164 0.90900 0.12025
C -3.37302 -0.48045 -0.14022
C -4.00858 0.00975 1.00418
C -5.35590 -0.26808 1.23266
C -6.07582 -1.03740 0.32027
C -5.44074 -1.53957 -0.81707
C -4.09474 -1.26756 -1.04176
C 0.38048 2.68047 0.00596
O -0.14903 3.79218 0.05173
H -2.05175 1.63423 0.40444
H 3.53536 0.54820 -1.33173
H 2.62239 -2.42613 1.61059
H 4.97333 -3.23439 1.53231
H 6.61591 -2.14245 0.00499
H 5.86428 -0.24761 -1.42718
H -3.44631 0.58183 1.73706
H -5.83969 0.10996 2.12881
H -7.12591 -1.25222 0.49848
H -5.99636 -2.14593 -1.52698
H -3.57340 -1.65867 -1.91021
C -1.92013 -0.22552 -0.45183
O -1.28519 -0.97603 -1.16989

33
SCF Energy = -989.289376561
Enthalpy 0K = -989.043331
Enthalpy 298K = -989.024989
Free Energy 298K = -989.088983
Lowest Frequencies = 49.2699 cm-1
ASQ1b_b
C -2.94483 1.65568 -1.40538
C -1.77555 1.34477 -2.09926
C -0.54229 1.34919 -1.45250
C -0.44399 1.65775 -0.07899
C -1.62981 2.00365 0.59938
C -2.85669 1.99111 -0.05034
N 0.75836 1.71532 0.60996
C 1.72275 0.90640 0.29567
C 3.18609 0.95331 0.69273
O 3.85212 1.66620 1.40383
C 1.99607 -0.31721 -0.40390
N 1.31625 -1.25953 -1.16324

C -0.80794 -1.46765 0.09902
C -0.26232 -1.32329 1.37772
C -1.10226 -1.15876 2.47732
C -2.48497 -1.13651 2.30671
C -3.03117 -1.29888 1.03261
C -2.19668 -1.47444 -0.06453
C 3.41400 -0.29195 -0.17230
O 4.36392 -0.97829 -0.53583
H 1.86849 -1.69756 -1.89684
H -1.55343 2.25666 1.65329
H 0.36349 1.12550 -2.00963
H -1.82061 1.08695 -3.15487
H -3.90695 1.64297 -1.91029
H -3.75869 2.23619 0.50660
H 0.81325 -1.33871 1.51978
H -0.67031 -1.03551 3.46610
H -3.13644 -0.98926 3.16426
H -4.10849 -1.27270 0.89281
H -2.59963 -1.60166 -1.06415
C 0.02330 -1.72215 -1.12265
O -0.41545 -2.39160 -2.05323

33
SCF Energy = -989.281553321
Enthalpy 0K = -989.035823
Enthalpy 298K = -989.016967
Free Energy 298K = -989.085483
Lowest Frequencies = 22.0819 cm-1
ASQ1b_c
C -5.43276 -2.16599 -0.11214
C -4.27238 -2.94180 -0.15881
C -3.01994 -2.33905 -0.13599
C -2.87506 -0.93783 -0.06564
C -4.05525 -0.16373 -0.01882
C -5.30478 -0.77692 -0.04268
N -1.57793 -0.44640 -0.04776
C -1.29129 0.82856 0.00785
C -1.83438 2.25365 0.07523
O -2.91662 2.79643 0.09224
C 0.01588 1.36874 0.03648
N 1.12080 0.54282 0.02765
C 3.41196 -0.25443 0.00021
C 3.11332 -1.49470 0.57299
C 4.07647 -2.50217 0.60738
C 5.34347 -2.27941 0.07060
C 5.64876 -1.03928 -0.49221
C 4.68988 -0.03125 -0.52031
C -0.38107 2.75742 0.13119
O 0.11380 3.86575 0.23054
H 0.85071 -0.43821 -0.01690
H -3.98663 0.91877 0.03418
H -2.11280 -2.93630 -0.17352
H -4.34395 -4.02604 -0.21404
H -6.41392 -2.63260 -0.12992
H -6.19557 -0.15349 -0.00606
H 2.14019 -1.67778 1.02037
H 3.83629 -3.45971 1.06046
H 6.09189 -3.06663 0.09668
H 6.63660 -0.85812 -0.90665
H 4.90630 0.94710 -0.93831
C 2.43700 0.89549 -0.06503
O 2.82431 2.04335 -0.20119

33
SCF Energy = -989.302064678
Enthalpy 0K = -989.055816
Enthalpy 298K = -989.037286
Free Energy 298K = -989.104626
Lowest Frequencies = 12.8871 cm-1
ASQ1c_a
C 5.38701 -2.03741 -0.00000
C 4.23139 -2.82060 -0.00002
C 2.97516 -2.22729 -0.00002
C 2.84508 -0.82614 -0.00000
C 4.00463 -0.03478 0.00002
C 5.25439 -0.64817 0.00002
N 1.55970 -0.30634 0.00000
C 1.12462 0.98006 0.00000
C 1.71598 2.33607 -0.00000
O 2.83209 2.82975 -0.00000
C -0.20195 1.48330 -0.00000
N -1.47443 1.07200 -0.00000
C -3.26218 -0.52095 0.00000
C -4.20658 0.51067 -0.00001
C -5.56824 0.21385 -0.00001
C -5.99892 -1.11396 -0.00000
C -5.05941 -2.14568 0.00001
C -3.69785 -1.84880 0.00001
C 0.29565 2.88029 -0.00000
O -0.20347 3.98512 -0.00001
H 0.76828 -0.96213 0.00001
H 3.91968 1.04784 0.00003
H 2.07673 -2.83987 -0.00003
H 4.30585 -3.90519 -0.00003

H 6.36931 -2.50055 -0.00000
H 6.14160 -0.01988 0.00003
H -3.84704 1.53437 -0.00001
H -6.29648 1.02083 -0.00002
H -7.06168 -1.34336 -0.00001
H -5.38923 -3.18156 0.00001
H -2.94713 -2.63299 0.00002
C -1.77789 -0.23640 0.00001
O -1.00388 -1.22006 0.00002

33
SCF Energy = -989.284068462
Enthalpy 0K = -989.038549
Enthalpy 298K = -989.019890
Free Energy 298K = -989.085600
Lowest Frequencies = 20.1441 cm-1
ASQ1c_b
C -3.20495 2.01524 -0.66436
C -2.07575 1.88262 -1.47190
C -0.81925 1.66706 -0.91450
C -0.68527 1.53862 0.47518
C -1.81748 1.68619 1.29120
C -3.06160 1.92787 0.72278
N 0.54649 1.26187 1.05625
C 1.65763 0.76361 0.43140
C 3.01740 0.85820 0.90589
O 3.53682 1.35823 1.89818
C 1.97623 -0.07670 -0.67578
N 1.42265 -0.70444 -1.68250
C -0.58271 -1.55628 -0.48123
C 0.11045 -2.06148 0.62118
C -0.58100 -2.46808 1.76290
C -1.97059 -2.36883 1.81296
C -2.66974 -1.88101 0.70682
C -1.97916 -1.48978 -0.43546
C 3.43868 0.05242 -0.32031
O 4.47340 -0.34705 -0.80210
H 0.70393 1.57889 2.00630
H -1.71551 1.56776 2.36740
H 0.05312 1.57264 -1.55382
H -2.16442 1.93549 -2.55323
H -4.18260 2.18197 -1.10680
H -3.93122 2.02467 1.36786
H 1.19293 -2.14109 0.58594
H -0.03060 -2.85866 2.61475
H -2.50708 -2.67279 2.70843
H -3.75303 -1.79601 0.73988
H -2.50158 -1.10406 -1.30583
C 0.11132 -1.07032 -1.74653
O -0.52687 -1.09954 -2.79714

33
SCF Energy = -989.289092798
Enthalpy 0K = -989.043281
Enthalpy 298K = -989.024463
Free Energy 298K = -989.092535
Lowest Frequencies = 21.9890 cm-1
ASQ1c_c
C -5.71356 -1.84111 -0.08348
C -4.64594 -2.72514 -0.24329
C -3.33642 -2.25885 -0.25012
C -3.06788 -0.88830 -0.09599
C -4.13785 0.00664 0.06444
C -5.44131 -0.48014 0.06847
N -1.75022 -0.46049 -0.10689
C -1.24382 0.80160 0.03021
C -1.66365 2.18909 0.20300
O -2.70949 2.81658 0.29066
C 0.12832 1.09848 0.01293
N 1.12500 0.22977 -0.06771
C 3.48335 -0.29571 -0.12301
C 3.25230 -1.53500 0.48022
C 4.31085 -2.41084 0.71827
C 5.61071 -2.05437 0.35718
C 5.84645 -0.81631 -0.24285
C 4.78736 0.05719 -0.48021
C -0.17297 2.55366 0.26856
O 0.43343 3.56846 0.50742
H -1.02336 -1.16192 -0.22192
H -3.94018 1.06996 0.18033
H -2.50892 -2.95357 -0.37581
H -4.83062 -3.78953 -0.36419
H -6.73640 -2.20547 -0.07806
H -6.25910 0.22489 0.19312
H 2.23497 -1.79241 0.75558
H 4.12249 -3.37290 1.18829
H 6.43602 -2.73711 0.54370
H 6.85758 -0.53261 -0.52394
H 4.94198 1.02756 -0.94246
C 2.36619 0.69291 -0.39167
O 2.63972 1.77439 -0.90912

40
SCF Energy = -1663.72412977

Enthalpy 0K = -1663.454016
Enthalpy 298K = -1663.427797
Free Energy 298K = -1663.517253
Lowest Frequencies = 2.8631 cm-1
ASQ2_a
C 5.63805 -1.01551 0.06989
C 4.55400 -1.89303 0.02461
C 3.26298 -1.39220 -0.01369
C 3.04377 -0.00672 -0.00718
C 4.12765 0.87241 0.03728
C 5.42124 0.35861 0.07408
N 1.70382 0.41289 -0.04060
C 1.17556 1.64422 -0.06357
C 1.67396 3.08508 -0.07878
O 2.73614 3.64039 -0.07330
C -0.14241 2.08608 -0.08509
N -1.41593 1.56979 -0.07861
C -3.20598 -0.08444 -0.05017
C -4.15465 0.77900 0.50909
C -5.49479 0.41193 0.53683
C -5.88332 -0.81534 0.00161
C -4.94463 -1.68603 -0.54630
C -3.60293 -1.32029 -0.56497
C 0.19757 3.50506 -0.09900
O -0.44716 4.52455 -0.11808
H -2.15088 2.26785 -0.13371
H 0.99755 -0.32332 -0.07153
H 3.97369 1.94508 0.04236
H 2.41609 -2.07253 -0.04607
H 4.72084 -2.96604 0.02324
H 6.26383 1.04094 0.11067
H -3.86144 1.72324 0.95914
H -6.23570 1.07374 0.97442
H -5.26044 -2.63892 -0.95699
H -2.84984 -1.98280 -0.97852
C -1.74773 0.23704 -0.10663
O -0.89541 -0.63658 -0.18709
C 7.02619 -1.58373 0.08339
F 7.95761 -0.65474 0.34749
F 7.15715 -2.55639 1.00595
F 7.35040 -2.14195 -1.10037
C -7.33665 -1.20460 0.07430
F -8.13805 -0.18019 -0.26076
F -7.62740 -2.22926 -0.73925
F -7.68024 -1.57502 1.32083

SCF Energy = -1663.72066287
Enthalpy 0K = -1663.450922
Enthalpy 298K = -1663.425089
Free Energy 298K = -1663.508146
Lowest Frequencies = 23.1141 cm-1
ASQ2_b
C -1.84694 -1.97035 -0.68139
C -0.64913 -2.52865 -0.24209
C 0.55877 -1.93187 -0.58567
C 0.55914 -0.76135 -1.35092
C -0.64270 -0.21644 -1.81150
C -1.84448 -0.82516 -1.47859
N 1.77057 -0.12025 -1.67088
C 2.90748 -0.18942 -0.95529
C 4.29551 0.08836 -1.42967
O 4.74594 0.46808 -2.47497
C 3.32871 -0.43295 0.34195
N 2.82627 -0.76228 1.56822
C 0.64262 0.44407 1.56647
C 1.10154 1.60755 0.94581
C 0.18837 2.53262 0.44562
C -1.17567 2.28677 0.57459
C -1.64190 1.14909 1.23517
C -0.72965 0.23445 1.74090
C 4.76573 -0.28531 -0.00503
O 5.78950 -0.43806 0.60355
H 3.47825 -1.24010 2.18836
H 1.85924 0.29627 -2.59279
H -0.63504 0.69832 -2.39786
H 1.49731 -2.37895 -0.27124
H -0.65551 -3.42962 0.36303
H -2.78155 -0.39437 -1.81864
H 2.16508 1.80853 0.86209
H 0.53637 3.43985 -0.03744
H -2.70859 0.97671 1.34339
H -1.06549 -0.65737 2.26095
C 1.56045 -0.58844 2.14086
O 1.26233 -1.24377 3.11665
C -3.15756 -2.55038 -0.23541
F -3.62744 -1.90877 0.85735
F -4.10541 -2.44088 -1.17979
F -3.05615 -3.84707 0.09116
C -2.16795 3.21633 -0.06735
F -1.67671 4.45291 -0.23278
F -2.51929 2.76895 -1.29408
F -3.29990 3.31873 0.64328

40
SCF Energy = -1663.70304668
Enthalpy 0K = -1663.434289
Enthalpy 298K = -1663.407655
Free Energy 298K = -1663.497612
Lowest Frequencies = 11.1500 cm-1
ASQ2_c

C	5.83839	-1.09130	0.06360
C	4.85129	-1.94195	0.55101
C	3.53143	-1.51022	0.59433
C	3.19374	-0.22903	0.14703
C	4.18429	0.62593	-0.34740
C	5.50119	0.18738	-0.38019
N	1.83685	0.13878	0.19646
C	1.26394	1.34183	-0.03713
C	1.69684	2.77865	-0.24204
O	2.73336	3.37324	-0.32843
C	-0.06968	1.68623	-0.11227
N	-1.21882	0.93338	-0.07814
C	-3.62219	0.59746	0.24388
C	-3.76047	-0.26205	-0.84721
C	-4.92695	-1.00854	-1.00544
C	-5.94545	-0.88879	-0.06634
C	-5.82127	-0.02025	1.02012
C	-4.66233	0.72767	1.17022
C	0.19241	3.12716	-0.34644
O	-0.44603	4.11412	-0.56797
H	-1.19410	-0.02994	-0.39020
H	1.21139	-0.59471	0.51180
H	3.93859	1.62667	-0.68279
H	2.76113	-2.17225	0.98215
H	5.10897	-2.93618	0.89939
H	6.27422	0.85039	-0.75767
H	-2.98570	-0.32786	-1.60616
H	-5.04560	-1.66942	-1.85698
H	-6.63089	0.06792	1.73850
H	-4.54326	1.42137	1.99627
C	-2.40248	1.43600	0.46833
O	-2.41276	2.46503	1.10203
C	7.27317	-1.52496	-0.00738
F	8.08264	-0.68254	0.66039
F	7.46123	-2.75077	0.50785
F	7.72225	-1.55504	-1.27694
C	-7.21556	-1.68604	-0.20003
F	-8.29035	-0.88568	-0.29939
F	-7.20676	-2.48239	-1.27889
F	-7.41559	-2.46929	0.87502

39
SCF Energy = -1663.20006755
Enthalpy 0K = -1662.944752
Enthalpy 298K = -1662.918500
Free Energy 298K = -1663.007737
Lowest Frequencies = 9.1172 cm-1
ASQ2b_a

C	5.66167	-0.97766	0.11484
C	4.72844	-1.67055	0.89209
C	3.40838	-1.25275	0.92596
C	2.97272	-0.12315	0.19864
C	3.92665	0.54677	-0.59866
C	5.24850	0.12693	-0.63363
N	1.62935	0.19132	0.25980
C	1.21368	1.40669	0.08015
C	1.76945	2.84475	0.07301
O	2.86242	3.35585	0.11245
C	-0.08862	1.97515	0.00696
N	-1.38380	1.48454	0.04752
C	-3.25770	-0.01100	-0.33173
C	-3.97243	0.41732	0.79144
C	-5.30614	0.05585	0.95281
C	-5.92657	-0.73692	-0.01164
C	-5.21894	-1.18367	-1.12665
C	-3.88464	-0.82270	-1.27937
C	0.32026	3.34246	0.05386
O	-0.25760	4.42520	0.10820
H	-2.08272	2.16908	0.31678
H	3.62146	1.40830	-1.18159
H	2.67068	-1.78333	1.52010
H	5.04214	-2.53551	1.47037
H	5.96813	0.66504	-1.24390
H	-3.48300	1.00914	1.55921
H	-5.86253	0.38481	1.82549
H	-5.70960	-1.80496	-1.86867
H	-3.30216	-1.16347	-2.12943
C	-1.80944	0.33689	-0.57173
O	-1.10377	-0.36064	-1.27503
C	7.06399	-1.47119	0.02704
F	7.94206	-0.50421	-0.31256
F	7.50379	-2.00298	1.19019
F	7.22535	-2.45248	-0.89858
C	-7.35419	-1.14706	0.20102
F	-8.11174	-0.12679	0.64910
F	-7.93315	-1.60441	-0.92288
F	-7.46630	-2.12916	1.12017

39
SCF Energy = -1663.21563641
Enthalpy 0K = -1662.959592
Enthalpy 298K = -1662.934002
Free Energy 298K = -1663.017369
Lowest Frequencies = 16.3436 cm-1
ASQ2b_b
C -1.72734 -2.00503 -0.69835
C -0.51222 -2.55220 -0.28698
C 0.68365 -1.93814 -0.63671
C 0.69709 -0.74787 -1.40065
C -0.54538 -0.24005 -1.84381
C -1.73545 -0.84762 -1.48780
N 1.84833 -0.10309 -1.79159
C 2.90519 -0.13151 -1.03128
C 4.33864 0.22672 -1.37265
O 4.89928 0.64305 -2.35507
C 3.31849 -0.36302 0.31777
N 2.77641 -0.75062 1.53416
C 0.58981 0.42085 1.50351
C 1.01859 1.57666 0.84709
C 0.08449 2.48888 0.36339
C -1.27377 2.24177 0.54125
C -1.71077 1.10327 1.22052
C -0.77647 0.20300 1.71075
C 4.72220 -0.15060 0.06508
O 5.74101 -0.25422 0.73422
H 3.41902 -1.25253 2.14358
H -0.53869 0.66018 -2.45126
H 1.62702 -2.38231 -0.33225
H -0.49974 -3.45667 0.31456
H -2.68101 -0.42014 -1.81205
H 2.07666 1.77008 0.70650
H 0.41500 3.38101 -0.15819
H -2.77248 0.91629 1.35092
H -1.08907 -0.68974 2.24264
C 1.53398 -0.58456 2.09593
O 1.22613 -1.20999 3.10373
C -3.01880 -2.59726 -0.25081
F -3.53911 -1.96157 0.83240
F -3.97940 -2.53152 -1.19876
F -2.90919 -3.89348 0.10319
C -2.28870 3.16693 -0.05958
F -1.81135 4.41272 -0.24031
F -2.70815 2.74006 -1.27059
F -3.39510 3.27799 0.70234

39
SCF Energy = -1663.20503595
Enthalpy 0K = -1662.949400
Enthalpy 298K = -1662.923237
Free Energy 298K = -1663.011595
Lowest Frequencies = 14.4287 cm-1
ASQ2b_c
C -5.32121 -1.33219 -0.06439
C -4.14729 -2.08629 -0.11000
C -2.91590 -1.44915 -0.09656
C -2.80562 -0.04246 -0.03449
C -4.00875 0.70405 0.01304
C -5.23756 0.06299 -0.00130
N -1.52919 0.47797 -0.02673
C -1.27534 1.76496 0.02435
C -1.85837 3.17305 0.09286
O -2.95414 3.68366 0.11710
C 0.01459 2.33255 0.04154
N 1.14172 1.53831 0.02435
C 3.45906 0.82110 -0.02638
C 3.21347 -0.42384 0.55645
C 4.21026 -1.39839 0.58353
C 5.45424 -1.12185 0.02609
C 5.71488 0.12412 -0.54913
C 4.72095 1.09198 -0.56700
C -0.41591 3.71568 0.13483
O 0.05511 4.83146 0.22585
H 0.90168 0.54937 -0.02005
H -3.96982 1.78810 0.05849
H -1.99568 -2.02431 -0.13682
H -4.19950 -3.16971 -0.16034
H -6.14954 0.65433 0.03362
H 2.25541 -0.64098 1.01957
H 4.01971 -2.36289 1.04174
H 6.69297 0.32962 -0.97510
H 4.89622 2.07555 -0.99091
C 2.44298 1.93694 -0.08022
O 2.79278 3.09537 -0.21688
C -6.66128 -1.98130 -0.05044
F -7.50677 -1.45572 -0.96793
F -6.60652 -3.30722 -0.29648
F -7.30156 -1.84770 1.13817
C 6.54939 -2.14729 0.03116
F 7.65366 -1.70124 0.66452
F 6.18783 -3.29186 0.63501
F 6.94173 -2.47015 -1.21837

39
SCF Energy = -1663.22615080
Enthalpy 0K = -1662.969867
Enthalpy 298K = -1662.944037
Free Energy 298K = -1663.031956
Lowest Frequencies = 7.3108 cm-1
ASQ2c_a

C	5.56057	-1.02716	0.02684
C	4.46014	-1.88961	0.01580
C	3.17568	-1.37661	0.00613
C	2.95800	0.01750	0.00555
C	4.06674	0.88071	0.01441
C	5.35162	0.35172	0.02311
N	1.64929	0.45106	-0.00140
C	1.13325	1.71131	-0.00123
C	1.64214	3.10106	0.00120
O	2.72476	3.65946	0.00391
C	-0.21918	2.12735	-0.00369
N	-1.46304	1.63479	-0.00677
C	-3.14200	-0.06746	-0.01388
C	-4.14819	0.90495	-0.01015
C	-5.48583	0.52652	-0.01641
C	-5.82208	-0.82898	-0.02833
C	-4.82818	-1.80574	-0.02897
C	-3.49044	-1.41943	-0.02341
C	0.18688	3.55630	-0.00128
O	-0.38238	4.62363	-0.00122
H	0.89948	-0.25295	-0.00551
H	3.91624	1.95605	0.01577
H	2.31866	-2.04485	0.00172
H	4.61336	-2.96538	0.01976
H	6.20169	1.02680	0.03232
H	-3.85441	1.94901	-0.00507
H	-6.26997	1.27839	-0.01834
H	-5.09892	-2.85673	-0.04050
H	-2.69273	-2.15498	-0.02833
C	-1.67763	0.31112	-0.01059
O	-0.84564	-0.62307	-0.01244
C	6.93475	-1.60549	0.00138
F	7.89079	-0.69776	0.27565
F	7.08681	-2.61247	0.89196
F	7.25560	-2.14107	-1.20180
C	-7.26889	-1.21618	0.00748
F	-8.02306	-0.45464	-0.81149
F	-7.47488	-2.49740	-0.35274
F	-7.80585	-1.07753	1.24059

39
SCF Energy = -1663.20828223
Enthalpy 0K = -1662.952568
Enthalpy 298K = -1662.926801
Free Energy 298K = -1663.010708
Lowest Frequencies = 13.3166 cm-1
ASQ2c_b

C	-1.98132	-1.94102	-0.64919
C	-0.81855	-2.51258	-0.13342
C	0.42484	-2.00165	-0.47856
C	0.51399	-0.88223	-1.32233
C	-0.66101	-0.32634	-1.85855
C	-1.89634	-0.85267	-1.52289
N	1.73728	-0.31400	-1.61922
C	2.89589	-0.43708	-0.89342
C	4.23151	-0.16045	-1.36746
O	4.69190	0.20590	-2.44068
C	3.28419	-0.64816	0.46098
N	2.80838	-0.93800	1.64454
C	0.69830	0.39651	1.56758
C	1.26081	1.53645	0.99052
C	0.44472	2.54783	0.48584
C	-0.93981	2.41921	0.56634
C	-1.51523	1.30448	1.18025
C	-0.69369	0.30805	1.68802
C	4.73004	-0.47439	0.04499
O	5.79186	-0.53011	0.61510
H	1.82504	0.21598	-2.47935
H	-0.59567	0.54982	-2.49850
H	1.32867	-2.45015	-0.07781
H	-0.87776	-3.35358	0.55045
H	-2.80139	-0.40118	-1.91927
H	2.33950	1.63694	0.92729
H	0.88487	3.42896	0.02916
H	-2.59577	1.21205	1.24509
H	-1.11229	-0.57317	2.16381
C	1.51925	-0.79382	2.05615
O	0.98738	-1.54910	2.86586
C	-3.32391	-2.42737	-0.21459
F	-3.83144	-1.69846	0.80895
F	-4.24223	-2.35591	-1.20290
F	-3.30417	-3.70472	0.20948
C	-1.82761	3.44436	-0.06840
F	-1.23634	4.64910	-0.18144
F	-2.19805	3.08762	-1.32132
F	-2.97226	3.63238	0.61710

39
SCF Energy = -1663.21264311
Enthalpy 0K = -1662.956856
Enthalpy 298K = -1662.930749
Free Energy 298K = -1663.018905
Lowest Frequencies = 10.4441 cm-1
ASQ2c_c
C -5.61235 -1.17117 -0.07724
C -4.53208 -2.02271 -0.30552
C -3.24114 -1.51622 -0.32328
C -3.00628 -0.14613 -0.10882
C -4.09833 0.71165 0.12274
C -5.38275 0.19147 0.13673
N -1.70923 0.31862 -0.13298
C -1.23706 1.59152 0.05190
C -1.69976 2.95418 0.30181
O -2.76233 3.53738 0.44613
C 0.12162 1.93242 0.01469
N 1.14692 1.10572 -0.13121
C 3.51935 0.67870 -0.28002
C 3.35387 -0.59786 0.25916
C 4.44961 -1.44405 0.42218
C 5.71655 -1.00525 0.04518
C 5.89517 0.27207 -0.49204
C 4.79769 1.10807 -0.65148
C -0.21779 3.36672 0.34404
O 0.36308 4.38634 0.61278
H -0.96520 -0.35365 -0.30174
H -3.92905 1.77405 0.28330
H -2.40056 -2.18058 -0.50643
H -4.69919 -3.08170 -0.47429
H -6.22297 0.85779 0.31283
H 2.35686 -0.91263 0.54706
H 4.32119 -2.43670 0.84139
H 6.88964 0.60294 -0.77970
H 4.89963 2.10739 -1.06268
C 2.35635 1.63514 -0.46646
O 2.57799 2.74912 -0.93482
C -7.00791 -1.69449 -0.01595
F -7.87258 -0.94636 -0.73517
F -7.11099 -2.95755 -0.47669
F -7.50484 -1.71066 1.24371
C 6.91750 -1.88721 0.19881
F 7.87142 -1.32140 0.96980
F 6.62733 -3.07762 0.75529
F 7.51215 -2.14988 -0.98600

46
SCF Energy = -2337.62298343
Enthalpy 0K = -2337.343272
Enthalpy 298K = -2337.309608
Free Energy 298K = -2337.417763
Lowest Frequencies = 7.5057 cm-1
ASQ3_a
C -5.66555 0.98522 0.23702
C -4.56396 1.82687 0.28490
C -3.27018 1.32736 0.16766
C -3.06489 -0.04290 -0.00006
C -4.16331 -0.91029 -0.04962
C -5.44048 -0.38115 0.06920
N -1.73420 -0.47505 -0.10211
C -1.23122 -1.70193 -0.30828
C -1.76687 -3.11224 -0.53241
O -2.84404 -3.63161 -0.59912
C 0.07385 -2.16500 -0.40607
N 1.36050 -1.68485 -0.33637
C 3.18197 -0.08168 -0.07984
C 4.12215 -1.02756 0.32035
C 5.47011 -0.67377 0.39245
C 5.88603 0.60936 0.06968
C 4.93262 1.55295 -0.31993
C 3.58898 1.22172 -0.38932
C -0.30024 -3.56003 -0.62913
O 0.31978 -4.57737 -0.80824
H 2.07692 -2.38444 -0.50467
H -1.01473 0.24569 -0.03353
H -4.02912 -1.97857 -0.18029
H -2.42254 2.00725 0.20939
H -6.67287 1.37612 0.33135
H 3.83123 -2.03360 0.61212
H 6.93671 0.87807 0.12316
H 2.84380 1.95511 -0.67912
C 1.71754 -0.37067 -0.17098
O 0.88554 0.52311 -0.11281
C -6.64098 -1.28990 -0.00012
F -6.30303 -2.58343 -0.01703
F -7.45836 -1.09588 1.05008
F -7.36951 -1.04734 -1.10478
C -4.73122 3.31308 0.45695
F -6.01185 3.66432 0.62672
F -4.04314 3.76321 1.52145
F -4.26669 3.98500 -0.61186
C 6.45607 -1.71288 0.86054

F 6.30532 -2.86258 0.18224
F 7.72260 -1.31062 0.70715
F 6.27506 -2.00157 2.15994
C 5.40857 2.93997 -0.66883
F 6.23921 2.91369 -1.72433
F 4.39571 3.76077 -0.96974
F 6.09049 3.48794 0.34986

46
SCF Energy = -2337.62233701
Enthalpy 0K = -2337.342945
Enthalpy 298K = -2337.309658
Free Energy 298K = -2337.411088
Lowest Frequencies = 15.7876 cm-1
ASQ3_b
C -2.05803 1.32979 1.18287
C -0.94283 2.09285 0.85252
C 0.35000 1.59797 0.99779
C 0.53440 0.29307 1.45964
C -0.57406 -0.48530 1.80339
C -1.85227 0.04215 1.67236
N 1.81656 -0.25400 1.61194
C 2.96450 0.18749 1.05612
C 4.34026 -0.03694 1.59682
O 4.75733 -0.63751 2.54614
C 3.43870 0.83941 -0.06891
N 3.01917 1.43662 -1.22314
C 0.96544 0.12426 -1.73664
C 1.41584 -1.12720 -1.32824
C 0.48878 -2.14163 -1.08685
C -0.87249 -1.92220 -1.25235
C -1.30572 -0.67191 -1.69941
C -0.39850 0.34261 -1.95814
C 4.85503 0.78023 0.38930
O 5.88065 1.22780 -0.04124
H 3.68565 2.09315 -1.62899
H 1.94531 -0.92471 2.36505
H -0.43393 -1.50343 2.15902
H 1.20443 2.22891 0.76408
H -3.05995 1.72613 1.06322
H 2.47553 -1.32711 -1.19821
H -1.59022 -2.70758 -1.03229
H -0.72807 1.31697 -2.30583
C 1.87386 1.28147 -2.00829
O 1.65191 2.07197 -2.89805
C -1.10051 3.48228 0.29234
F -0.71317 3.52431 -0.99699
F -2.36523 3.91233 0.34707
F -0.33631 4.36683 0.95318
C -3.01306 -0.81900 2.10042
F -2.91720 -2.05786 1.58488
F -3.03706 -0.96089 3.43787
F -4.19050 -0.30857 1.72999
C -2.77907 -0.43846 -1.90958
F -3.20836 -0.98859 -3.05569
F -3.50273 -0.98309 -0.91715
F -3.07555 0.86856 -1.95487
C 0.97283 -3.45247 -0.53041
F 2.18461 -3.77922 -0.99852
F 1.08163 -3.38585 0.81681
F 0.13691 -4.46014 -0.80338

46
SCF Energy = -2337.60219830
Enthalpy 0K = -2337.323832
Enthalpy 298K = -2337.289793
Free Energy 298K = -2337.398316
Lowest Frequencies = 6.9139 cm-1
ASQ3_c
C 5.95550 0.85113 -0.05716
C 5.04097 1.72565 -0.64187
C 3.69617 1.40213 -0.73624
C 3.23912 0.18226 -0.22457
C 4.13450 -0.69826 0.37998
C 5.48304 -0.35408 0.44468
N 1.86225 -0.09246 -0.30640
C 1.25618 -1.29952 -0.21691
C 1.69045 -2.74835 -0.25089
O 2.73251 -3.33411 -0.31018
C -0.07451 -1.64559 -0.14602
N -1.22468 -0.90111 -0.03145
C -3.64208 -0.55358 -0.21273
C -3.74295 0.15033 0.98663
C -4.91308 0.84557 1.28311
C -5.98663 0.84669 0.39952
C -5.87904 0.12912 -0.78997
C -4.72162 -0.57609 -1.09761
C 0.18696 -3.11004 -0.13348
O -0.45471 -4.11329 -0.03615
H -1.18551 0.01127 0.40718
H 1.27470 0.69662 -0.55150
H 3.79999 -1.64481 0.78891
H 3.00467 2.09487 -1.20714
H 7.00594 1.11224 0.01481

H -2.93676 0.13905 1.71594
H -6.89220 1.39568 0.63302
H -4.63853 -1.14750 -2.01820
C -2.42255 -1.33130 -0.60356
O -2.45579 -2.25460 -1.38149
C -7.02457 0.08932 -1.76936
F -7.53764 -1.14648 -1.86903
F -8.01960 0.91282 -1.41243
F -6.62303 0.44707 -2.99983
C -4.99341 1.57472 2.59835
F -5.00477 0.71765 3.63238
F -3.92570 2.37575 2.77361
F -6.08985 2.33551 2.69038
C 5.54910 3.02725 -1.20364
F 6.30216 2.82789 -2.29793
F 4.54892 3.85216 -1.55284
F 6.31691 3.67776 -0.31545
C 6.43874 -1.34291 1.06367
F 6.71243 -2.35036 0.22117
F 7.60574 -0.76943 1.39329
F 5.92629 -1.88845 2.17814

45
SCF Energy = -2337.11120874
Enthalpy 0K = -2336.846192
Enthalpy 298K = -2336.812555
Free Energy 298K = -2336.920336
Lowest Frequencies = 8.6117 cm-1
ASQ3b_a
C -5.68752 0.93924 0.03676
C -4.75715 1.62906 0.80472
C -3.42920 1.21924 0.87982
C -2.98279 0.07421 0.19770
C -3.92508 -0.61407 -0.60222
C -5.24086 -0.18322 -0.66548
N -1.64363 -0.24671 0.28562
C -1.25408 -1.48100 0.18643
C -1.85699 -2.89431 0.27317
O -2.96925 -3.35531 0.34816
C 0.02793 -2.08981 0.15532
N 1.33466 -1.62720 0.16260
C 3.22253 -0.17987 -0.32551
C 3.93241 -0.51597 0.82294
C 5.27136 -0.13525 0.95084
C 5.90761 0.57823 -0.05289
C 5.18200 0.92229 -1.19656
C 3.85162 0.55844 -1.33525
C -0.42268 -3.44115 0.28514
O 0.12009 -4.53383 0.40641
H 2.02108 -2.30363 0.48066
H -3.61360 -1.48576 -1.16554
H -2.70823 1.77396 1.47333
H -6.71995 1.26423 -0.02694
H 3.44750 -1.04642 1.63840
H 6.94794 0.87048 0.04896
H 3.27272 0.83675 -2.21015
C 1.77199 -0.53546 -0.54017
O 1.07763 0.11788 -1.29443
C -6.24397 -0.91709 -1.50690
F -5.71113 -1.92767 -2.20690
F -7.24415 -1.43656 -0.76263
F -6.84361 -0.09632 -2.40118
C -5.16159 2.85596 1.56657
F -6.47481 3.13253 1.45233
F -4.90386 2.74596 2.88661
F -4.49931 3.95637 1.15086
C 6.00061 -0.50350 2.21267
F 5.97685 -1.83109 2.42986
F 7.29030 -0.12871 2.18608
F 5.44308 0.07046 3.29412
C 5.89061 1.70488 -2.26670
F 6.97758 1.04777 -2.71957
F 5.11048 1.95957 -3.32390
F 6.33491 2.88910 -1.80122

45
SCF Energy = -2337.12735296
Enthalpy 0K = -2336.861644
Enthalpy 298K = -2336.828654
Free Energy 298K = -2336.929438
Lowest Frequencies = 19.1832 cm-1
ASQ3b_b
C -1.76914 1.70066 1.04205
C -0.59998 2.37790 0.69791
C 0.65634 1.82758 0.91534
C 0.78753 0.54013 1.48978
C -0.39565 -0.12068 1.87749
C -1.63919 0.44953 1.64304
N 1.99092 -0.06759 1.74989
C 3.03195 0.18655 1.00448
C 4.49696 -0.08874 1.28738
O 5.10543 -0.59652 2.19292
C 3.39867 0.67380 -0.28437
N 2.80723 1.20713 -1.41962

C 0.70984 -0.11453 -1.56512
C 1.21116 -1.31622 -1.05687
C 0.32793 -2.33780 -0.72614
C -1.04605 -2.18995 -0.90092
C -1.52947 -1.00323 -1.44136
C -0.66130 0.02958 -1.77930
C 4.82339 0.54943 -0.07301
O 5.81348 0.85418 -0.71818
H 3.39880 1.85001 -1.94298
H -0.30543 -1.09848 2.34255
H 1.54751 2.39021 0.65572
H -2.74501 2.13215 0.84719
H 2.27674 -1.45941 -0.91577
H -1.72701 -2.98649 -0.61688
H -1.03080 0.95970 -2.20224
C 1.57614 1.03328 -2.00047
O 1.20631 1.77360 -2.90216
C -0.73891 3.72292 0.04394
F -1.35528 3.63441 -1.15243
F -1.48910 4.56694 0.78649
F 0.43905 4.32937 -0.16359
C -2.86314 -0.29546 2.09261
F -2.77333 -1.61674 1.84415
F -3.06784 -0.17627 3.42224
F -3.98384 0.14253 1.49283
C -2.99747 -0.84104 -1.72020
F -3.28101 -1.07133 -3.02100
F -3.74970 -1.69417 -1.00694
F -3.42929 0.40132 -1.45206
C 0.83091 -3.62351 -0.13275
F 2.16610 -3.71217 -0.14887
F 0.43036 -3.77242 1.14273
F 0.35313 -4.69544 -0.80369

45
SCF Energy = -2337.11510158
Enthalpy 0K = -2336.849838
Enthalpy 298K = -2336.816256
Free Energy 298K = -2336.924222
Lowest Frequencies = 7.7994 cm-1
ASQ3b_c
C 5.45454 1.10701 -0.30532
C 4.28756 1.86802 -0.40576
C 3.03446 1.28954 -0.29324
C 2.88375 -0.09965 -0.07614
C 4.06293 -0.86879 0.02543
C 5.31034 -0.25893 -0.08801
N 1.59160 -0.56591 0.01549
C 1.29808 -1.83152 0.20846
C 1.84942 -3.23887 0.41207
O 2.93441 -3.76779 0.45871
C -0.00277 -2.35607 0.31637
N -1.11784 -1.54559 0.24933
C -3.43546 -0.83159 0.12386
C -3.19954 0.44833 0.63723
C -4.20718 1.40521 0.59362
C -5.45499 1.11299 0.04441
C -5.68315 -0.16414 -0.45171
C -4.68652 -1.13701 -0.40699
C 0.39431 -3.73324 0.55530
O -0.10485 -4.81339 0.79040
H -0.86747 -0.56665 0.12054
H 4.00183 -1.94165 0.19288
H 2.13453 1.88990 -0.37373
H 6.43315 1.56506 -0.39318
H -2.24783 0.70112 1.09431
H -6.23352 1.86849 0.01284
H -4.86095 -2.14493 -0.77389
C -2.41728 -1.94725 0.14292
O -2.77053 -3.10862 0.05969
C -7.01064 -0.52321 -1.05997
F -7.54491 -1.61268 -0.48242
F -7.91022 0.46930 -0.94433
F -6.89699 -0.80049 -2.37185
C -3.99355 2.77912 1.16569
F -4.77486 2.99249 2.24342
F -2.72710 2.98698 1.54735
F -4.30921 3.73925 0.27546
C 4.42554 3.34828 -0.60185
F 5.30394 3.65053 -1.58188
F 3.26578 3.94821 -0.92102
F 4.88565 3.96791 0.50816
C 6.53158 -1.13145 -0.01275
F 6.68642 -1.88274 -1.12242
F 7.66803 -0.41552 0.12192
F 6.48713 -1.98693 1.02255

45
SCF Energy = -2337.13658024
Enthalpy 0K = -2336.870718
Enthalpy 298K = -2336.837435
Free Energy 298K = -2336.945125
Lowest Frequencies = 5.9428 cm-1
ASQ3c_a

C -5.59627 0.98853 0.00066
C -4.48405 1.81996 0.00516
C -3.19192 1.30569 0.00782
C -2.98081 -0.08202 0.00624
C -4.09912 -0.93952 0.00226
C -5.37194 -0.38997 -0.00027
N -1.67816 -0.53016 0.00890
C -1.17993 -1.79876 0.00697
C -1.71541 -3.17877 0.00491
O -2.81004 -3.71041 0.00444
C 0.16241 -2.23781 0.00602
N 1.41456 -1.76293 0.00562
C 3.11204 -0.08518 0.00757
C 4.10290 -1.06406 -0.00543
C 5.44789 -0.68945 -0.01019
C 5.81893 0.64911 -0.00068
C 4.81774 1.62132 0.01315
C 3.47498 1.26507 0.01619
C -0.26681 -3.66117 0.00354
O 0.28419 -4.73610 0.00138
H -0.91926 0.16456 0.01301
H -3.96077 -2.01804 0.00169
H -2.33726 1.97783 0.01190
H -6.60237 1.39224 -0.00088
H 3.80186 -2.10781 -0.01237
H 6.86597 0.93509 -0.00314
H 2.68777 2.01154 0.02697
C 1.64282 -0.44438 0.01147
O 0.82871 0.50487 0.01990
C -6.57929 -1.28600 -0.00225
F -6.27135 -2.58583 -0.01166
F -7.35910 -1.06797 1.07956
F -7.36606 -1.05392 -1.07608
C -4.64711 3.31286 -0.00701
F -5.93494 3.69250 0.06625
F -4.00643 3.89945 1.02295
F -4.14105 3.86558 -1.12777
C 6.49286 -1.76847 -0.01273
F 6.33744 -2.61741 -1.04430
F 7.74262 -1.27262 -0.09830
F 6.44732 -2.51544 1.10646
C 5.23794 3.06210 0.00627
F 5.87443 3.39404 -1.13775
F 4.20571 3.90689 0.13820
F 6.10465 3.33639 1.00437

45

SCF Energy = -2337.11871659
Enthalpy 0K = -2336.853459
Enthalpy 298K = -2336.820255
Free Energy 298K = -2336.921808
Lowest Frequencies = 14.7621 cm-1
ASQ3c_b
C -2.07924 1.48511 0.98220
C -0.99530 2.26477 0.57784
C 0.31539 1.87163 0.80290
C 0.56836 0.63788 1.43153
C -0.51213 -0.14657 1.85777
C -1.81397 0.28552 1.63464
N 1.85728 0.18583 1.62149
C 2.98486 0.60812 0.95619
C 4.35012 0.46297 1.41131
O 4.86402 0.01058 2.42242
C 3.32929 1.09862 -0.33362
N 2.81378 1.51765 -1.46119
C 0.84170 -0.01756 -1.62878
C 1.48310 -1.16017 -1.15616
C 0.73481 -2.29251 -0.82884
C -0.64555 -2.31511 -0.98802
C -1.27322 -1.18523 -1.51233
C -0.54209 -0.04974 -1.83407
C 4.79023 1.06838 0.07268
O 5.82625 1.36808 -0.46357
H 2.02473 -0.48253 2.36626
H -0.32633 -1.10796 2.33026
H 1.14083 2.50174 0.48503
H -3.09764 1.80446 0.78942
H 2.56059 -1.17111 -1.02517
H -1.22300 -3.19089 -0.70914
H -1.02208 0.84312 -2.22482
C 1.54610 1.31115 -1.90387
O 0.93031 2.12833 -2.58133
C -1.28934 3.55870 -0.13294
F -1.86804 3.34647 -1.32725
F -2.16211 4.31191 0.57732
F -0.19936 4.30314 -0.33084
C -2.94486 -0.55508 2.15644
F -2.70351 -1.87145 2.01756
F -3.14864 -0.34672 3.47618
F -4.10811 -0.29150 1.54266
C -2.75391 -1.21983 -1.76211
F -3.04460 -1.73939 -2.97479
F -3.39899 -1.98276 -0.86018
F -3.30993 0.00064 -1.72379

C 1.42488 -3.46732 -0.20006
F 2.66578 -3.64833 -0.67642
F 1.54377 -3.31240 1.13809
F 0.75212 -4.61845 -0.38857

45
SCF Energy = -2337.12278043
Enthalpy 0K = -2336.857453
Enthalpy 298K = -2336.823847
Free Energy 298K = -2336.933210
Lowest Frequencies = 6.0467 cm-1
ASQ3c_c
C 5.68941 0.90650 -0.19544
C 4.61568 1.77211 -0.40936
C 3.30604 1.32351 -0.38324
C 3.03037 -0.03499 -0.13671
C 4.09697 -0.91964 0.07974
C 5.40075 -0.43116 0.04602
N 1.71659 -0.44912 -0.11675
C 1.20922 -1.70361 0.10133
C 1.64633 -3.07321 0.36484
O 2.69942 -3.67365 0.49365
C -0.15549 -2.01066 0.10361
N -1.16690 -1.16247 -0.03248
C -3.52308 -0.67660 -0.15263
C -3.31223 0.60856 0.34502
C -4.38736 1.48291 0.49581
C -5.68135 1.09591 0.15941
C -5.88196 -0.19075 -0.33473
C -4.81671 -1.07422 -0.48982
C 0.15459 -3.44886 0.44820
O -0.44581 -4.44745 0.74548
H 0.99413 0.24759 -0.27848
H 3.90451 -1.97608 0.26836
H 2.48904 2.01841 -0.55261
H 6.71113 1.26774 -0.21724
H -2.30183 0.90645 0.60780
H -6.51313 1.78086 0.27693
H -4.96047 -2.08095 -0.87345
C -2.39128 -1.67186 -0.33137
O -2.65990 -2.78993 -0.76163
C -7.26336 -0.65862 -0.69175
F -7.70070 -1.62346 0.14098
F -8.17189 0.33473 -0.64368
F -7.31570 -1.17727 -1.93247
C -4.11888 2.85861 1.03306
F -3.57417 2.82175 2.26442
F -3.25300 3.54211 0.25885
F -5.23501 3.60591 1.12245
C 4.91838 3.21848 -0.67637
F 5.66686 3.37660 -1.78688
F 3.81175 3.96152 -0.84224
F 5.62008 3.77755 0.32991
C 6.51901 -1.41029 0.28406
F 6.52218 -2.39948 -0.62520
F 7.73093 -0.82291 0.22652
F 6.42631 -1.99344 1.49126

38
SCF Energy = -1398.67996206
Enthalpy 0K = -1398.413942
Enthalpy 298K = -1398.389977
Free Energy 298K = -1398.470925
Lowest Frequencies = 17.3513 cm-1
ASQ4_a
C 5.58257 -1.23107 0.07929
C 4.50772 -2.11329 0.06450
C 3.22430 -1.59404 0.02566
C 3.02025 -0.20537 0.00257
C 4.11466 0.66724 0.01824
C 5.40180 0.14655 0.05650
N 1.68849 0.22686 -0.03212
C 1.17304 1.46577 -0.07598
C 1.68862 2.90067 -0.11935
O 2.75654 3.44313 -0.12751
C -0.13905 1.91977 -0.10117
N -1.41842 1.41875 -0.08134
C -3.22639 -0.21558 -0.02084
C -4.16024 0.66159 0.54099
C -5.50655 0.31481 0.58096
C -5.88556 -0.91071 0.05028
C -4.97959 -1.80678 -0.50349
C -3.63666 -1.45184 -0.52894
C 0.21584 3.33663 -0.14243
O -0.41885 4.36049 -0.17805
H -2.14559 2.12414 -0.14941
H 0.97368 -0.50175 -0.04534
H 3.97032 1.74100 -0.00126
H 2.37003 -2.26530 0.01370
H 4.68461 -3.18204 0.08324
H 6.26475 0.80196 0.06879
H -3.85244 1.60304 0.98661
H -6.25141 0.96890 1.01812
H -5.32859 -2.75345 -0.89837

H -2.89211 -2.12455 -0.94105
C -1.76364 0.08973 -0.08296
O -0.92251 -0.79535 -0.14555
N 6.94494 -1.77285 0.12036
O 7.06922 -2.98575 0.13955
O 7.86917 -0.97889 0.13283
N -7.31626 -1.28165 0.08582
O -7.62540 -2.35754 -0.38937
O -8.08705 -0.48538 0.58721

38
SCF Energy = -1398.67358925
Enthalpy 0K = -1398.408267
Enthalpy 298K = -1398.384430
Free Energy 298K = -1398.463189
Lowest Frequencies = 24.9639 cm-1
ASQ4_b
C -2.15797 -1.94223 -0.69640
C -0.97618 -2.48942 -0.21205
C 0.22705 -1.88309 -0.54718
C 0.22802 -0.73198 -1.34601
C -0.97299 -0.21217 -1.84354
C -2.17652 -0.82078 -1.52008
N 1.43372 -0.09096 -1.66658
C 2.57782 -0.16115 -0.95715
C 3.96392 0.10241 -1.44766
O 4.40759 0.46654 -2.50017
C 3.00539 -0.38943 0.33921
N 2.51061 -0.69394 1.57467
C 0.33304 0.52355 1.55523
C 0.79741 1.67778 0.91963
C -0.10900 2.59768 0.40040
C -1.46465 2.33225 0.53432
C -1.95494 1.21512 1.20273
C -1.03998 0.31360 1.72748
C 4.44353 -0.25474 -0.02013
O 5.46850 -0.40481 0.58439
H 3.16521 -1.16067 2.20094
H 1.51520 0.33563 -2.58485
H -0.96055 0.68302 -2.45933
H 1.16397 -2.31217 -0.20518
H -1.00638 -3.37585 0.41117
H -3.12246 -0.42819 -1.87598
H 1.86143 1.87577 0.83737
H 0.21893 3.50151 -0.09933
H -3.02462 1.06361 1.29357
H -1.37448 -0.56988 2.26240
C 1.25059 -0.49896 2.15198
O 0.95299 -1.12344 3.14671
N -2.42917 3.27345 -0.06960
O -1.97753 4.24653 -0.64548
O -3.61153 3.00668 0.03461
N -3.43489 -2.56761 -0.32177
O -4.45526 -2.06469 -0.75659
O -3.39043 -3.54306 0.40622

38
SCF Energy = -1398.65887353
Enthalpy 0K = -1398.394263
Enthalpy 298K = -1398.369841
Free Energy 298K = -1398.452990
Lowest Frequencies = 11.8263 cm-1
ASQ4_c
C 5.83422 -1.23152 0.05436
C 4.86649 -2.11107 0.52589
C 3.54867 -1.68591 0.56861
C 3.20613 -0.39475 0.14139
C 4.19317 0.47644 -0.33254
C 5.51515 0.05236 -0.37061
N 1.85002 -0.03914 0.19239
C 1.26632 1.16167 -0.03865
C 1.68866 2.60390 -0.23353
O 2.72010 3.20699 -0.31198
C -0.06909 1.49351 -0.11660
N -1.21481 0.73507 -0.09036
C -3.61964 0.39491 0.22474
C -3.75890 -0.44691 -0.88298
C -4.92076 -1.19370 -1.05108
C -5.92004 -1.07677 -0.09442
C -5.81599 -0.23680 1.00803
C -4.65342 0.50889 1.15875
C 0.18096 2.93991 -0.34134
O -0.46682 3.92040 -0.55968
H -1.18631 -0.22658 -0.40754
H 1.22982 -0.77859 0.50440
H 3.94231 1.48154 -0.65043
H 2.77975 -2.35872 0.93942
H 5.15112 -3.10446 0.85162
H 6.29819 0.71008 -0.72927
H -2.98685 -0.49691 -1.64552
H -5.06340 -1.84589 -1.90436
H -6.63095 -0.17587 1.71944
H -4.53141 1.18939 1.99514
C -2.39988 1.23342 0.45645

O -2.41465 2.25835 1.09556
N -7.15165 -1.87604 -0.26266
O -7.21805 -2.60261 -1.23670
O -8.01563 -1.75660 0.58484
N 7.23198 -1.67507 0.00523
O 7.47688 -2.80752 0.38475
O 8.06024 -0.88567 -0.41231

37
SCF Energy = -1398.16704552
Enthalpy 0K = -1397.915617
Enthalpy 298K = -1397.891609
Free Energy 298K = -1397.973695
Lowest Frequencies = 10.2474 cm-1
ASQ4b_a
C 5.59319 -1.19577 0.08306
C 4.68407 -1.86491 0.90844
C 3.38004 -1.41647 0.97128
C 2.94581 -0.28401 0.23752
C 3.89203 0.35588 -0.60296
C 5.19867 -0.08899 -0.67395
N 1.62091 0.05513 0.33275
C 1.20870 1.26856 0.10489
C 1.77770 2.69829 0.05071
O 2.87464 3.19847 0.07241
C -0.08746 1.83664 0.01991
N -1.38384 1.35456 0.07144
C -3.25631 -0.15344 -0.26912
C -3.98388 0.32161 0.82687
C -5.32048 -0.02890 0.98995
C -5.90486 -0.85969 0.04199
C -5.20304 -1.36046 -1.05033
C -3.86875 -1.00440 -1.19472
C 0.33017 3.20664 0.01676
O -0.24285 4.28971 0.03260
H -2.08320 2.05340 0.30019
H 3.58573 1.21236 -1.19226
H 2.64764 -1.92189 1.59256
H 5.01462 -2.72507 1.47907
H 5.92324 0.40571 -1.31045
H -3.50306 0.94181 1.57716
H -5.90255 0.32110 1.83394
H -5.70076 -2.01205 -1.75846
H -3.27318 -1.38094 -2.02000
C -1.80347 0.17971 -0.50080
O -1.08954 -0.55094 -1.15924
N 6.95848 -1.66342 0.00413
O 7.28340 -2.63414 0.68207
O 7.73764 -1.07247 -0.73665
N -7.31904 -1.23192 0.20631
O -7.81623 -1.95948 -0.63630
O -7.91413 -0.79073 1.17495

37
SCF Energy = -1398.18034383
Enthalpy 0K = -1397.928301
Enthalpy 298K = -1397.904849
Free Energy 298K = -1397.982369
Lowest Frequencies = 28.9357 cm-1
ASQ4b_b
C -2.01475 -1.98206 -0.72972
C -0.80771 -2.51615 -0.27687
C 0.37832 -1.88711 -0.61152
C 0.38774 -0.70647 -1.40242
C -0.85762 -0.23070 -1.88851
C -2.04425 -0.84477 -1.54727
N 1.52441 -0.04778 -1.77268
C 2.59149 -0.08508 -1.01747
C 4.02507 0.25240 -1.37405
O 4.58529 0.64155 -2.36608
C 2.99912 -0.29611 0.33030
N 2.45912 -0.65106 1.55495
C 0.25360 0.48580 1.48478
C 0.67375 1.63857 0.81529
C -0.26475 2.53479 0.31418
C -1.61184 2.25243 0.49723
C -2.05919 1.12410 1.17904
C -1.11133 0.24778 1.68540
C 4.40961 -0.10127 0.07138
O 5.42291 -0.20385 0.74329
H 3.10707 -1.12512 2.18133
H -0.84773 0.65421 -2.51776
H 1.32231 -2.30866 -0.27913
H -0.81557 -3.40827 0.33948
H -2.99870 -0.45906 -1.88852
H 1.73009 1.84335 0.67891
H 0.03542 3.42862 -0.21883
H -3.12179 0.94190 1.28984
H -1.41167 -0.64331 2.22721
C 1.20955 -0.49139 2.10624
O 0.90642 -1.09105 3.12881
N -2.60806 3.18434 -0.05338
O -2.20082 4.17154 -0.64356
O -3.78712 2.91966 0.11127

N -3.25964 -2.61544 -0.34815
O -4.30872 -2.12005 -0.74500
O -3.21186 -3.61562 0.35953

37
SCF Energy = -1398.17191809
Enthalpy 0K = -1397.920139
Enthalpy 298K = -1397.896237
Free Energy 298K = -1397.977822
Lowest Frequencies = 16.7156 cm-1
ASQ4b_c
C 5.33420 -1.52885 0.07268
C 4.17390 -2.30748 0.12682
C 2.94534 -1.67959 0.10967
C 2.82556 -0.26730 0.03830
C 4.02577 0.49059 -0.01443
C 5.25923 -0.13451 0.00269
N 1.55263 0.23730 0.02626
C 1.28444 1.52634 -0.03305
C 1.85537 2.93798 -0.10841
O 2.94439 3.45912 -0.13353
C -0.00970 2.07299 -0.05620
N -1.13064 1.27241 -0.03787
C -3.45034 0.56027 0.02335
C -3.21011 -0.68403 -0.56958
C -4.20498 -1.65623 -0.59374
C -5.43390 -1.35845 -0.01794
C -5.70701 -0.12682 0.56849
C -4.70480 0.83416 0.57793
C 0.40527 3.46518 -0.15645
O -0.08135 4.57058 -0.25572
H -0.88862 0.28418 0.01179
H 3.97757 1.57361 -0.06779
H 2.02822 -2.25881 0.15207
H 4.25718 -3.38680 0.18167
H 6.17479 0.44472 -0.03772
H -2.25686 -0.89957 -1.04268
H -4.04298 -2.62408 -1.05269
H -6.68315 0.06108 0.99930
H -4.87275 1.81628 1.00760
C -2.43174 1.67382 0.07050
O -2.77825 2.83239 0.20533
N -6.49020 -2.38276 -0.03875
O -6.23533 -3.45138 -0.56754
O -7.56069 -2.10455 0.47457
N 6.62536 -2.17611 0.08967
O 6.66298 -3.40202 0.15173
O 7.63167 -1.47603 0.04136

37
SCF Energy = -1398.19283420
Enthalpy 0K = -1397.940392
Enthalpy 298K = -1397.916841
Free Energy 298K = -1397.997058
Lowest Frequencies = 9.5593 cm-1
ASQ4c_a
C 5.49725 -1.25375 -0.00001
C 4.39908 -2.11623 0.00001
C 3.12646 -1.58161 0.00002
C 2.92862 -0.18136 0.00001
C 4.05147 0.67193 -0.00001
C 5.32577 0.13133 -0.00002
N 1.63275 0.26812 0.00002
C 1.13129 1.53743 0.00001
C 1.65867 2.92102 0.00001
O 2.74669 3.46494 0.00001
C -0.21514 1.96668 0.00001
N -1.46406 1.48906 0.00001
C -3.15972 -0.19497 0.00002
C -4.15418 0.78973 -0.00002
C -5.49743 0.43169 -0.00003
C -5.82368 -0.92166 -0.00001
C -4.85739 -1.92288 0.00002
C -3.51956 -1.54641 0.00003
C 0.20625 3.39371 0.00000
O -0.35203 4.46472 -0.00000
H 0.87191 -0.42538 0.00003
H 3.91350 1.74882 -0.00002
H 2.25956 -2.23652 0.00004
H 4.55817 -3.18808 0.00002
H 6.19714 0.77590 -0.00004
H -3.84886 1.83025 -0.00003
H -6.28504 1.17569 -0.00005
H -5.15925 -2.96341 0.00004
H -2.72871 -2.28889 0.00006
C -1.69139 0.16786 0.00003
O -0.87013 -0.77501 0.00005
N 6.83587 -1.80994 -0.00002
O 6.95583 -3.02981 -0.00001
O 7.78556 -1.03691 -0.00004
N -7.24071 -1.30860 -0.00002
O -7.50914 -2.49989 0.00000
O -8.07722 -0.41978 -0.00006

37
SCF Energy = -1398.17197433
Enthalpy 0K = -1397.920284
Enthalpy 298K = -1397.896600
Free Energy 298K = -1397.975292
Lowest Frequencies = 16.9704 cm-1
ASQ4c_b
C -2.37863 -1.95332 -0.58001
C -1.24160 -2.46853 0.04068
C 0.00488 -1.98115 -0.31216
C 0.11652 -0.95477 -1.27101
C -1.04650 -0.46751 -1.90338
C -2.28931 -0.96188 -1.56029
N 1.33806 -0.41845 -1.59510
C 2.50967 -0.53148 -0.88186
C 3.84421 -0.34339 -1.40292
O 4.29533 -0.07459 -2.50614
C 2.91685 -0.65738 0.47593
N 2.45198 -0.83298 1.68494
C 0.42368 0.60718 1.51791
C 1.06353 1.69154 0.91123
C 0.32115 2.73303 0.36137
C -1.06545 2.66624 0.43140
C -1.73309 1.61605 1.05689
C -0.97379 0.59444 1.60958
C 4.36200 -0.57234 0.02263
O 5.43021 -0.63006 0.57644
H 1.42492 0.06995 -2.48031
H -0.96032 0.32899 -2.63764
H 0.89632 -2.38190 0.15935
H -1.33996 -3.23881 0.79693
H -3.19290 -0.58204 -2.02248
H 2.14721 1.72618 0.86786
H 0.79816 3.58051 -0.11639
H -2.81622 1.60781 1.09379
H -1.44665 -0.24553 2.10869
C 1.17527 -0.59211 2.09059
O 0.60551 -1.25073 2.95433
N -1.85548 3.75028 -0.16855
O -1.25459 4.65804 -0.72147
O -3.07116 3.68501 -0.08589
N -3.68834 -2.46760 -0.21313
O -4.66939 -1.99858 -0.77651
O -3.74722 -3.34301 0.63844

37
SCF Energy = -1398.17898596
Enthalpy 0K = -1397.927104
Enthalpy 298K = -1397.903231
Free Energy 298K = -1397.984505
Lowest Frequencies = 14.8013 cm-1
ASQ4c_c
C 5.61076 -1.33330 0.06307
C 4.54683 -2.20832 0.28604
C 3.25910 -1.70917 0.29955
C 3.01761 -0.33375 0.09122
C 4.10567 0.53542 -0.13142
C 5.39383 0.03020 -0.14397
N 1.72270 0.11752 0.11145
C 1.23829 1.38949 -0.06381
C 1.69114 2.75803 -0.30378
O 2.74751 3.34965 -0.44444
C -0.12263 1.71616 -0.02384
N -1.14259 0.88268 0.11530
C -3.51369 0.44873 0.25911
C -3.34037 -0.82716 -0.28671
C -4.42860 -1.67580 -0.45817
C -5.68786 -1.22236 -0.07720
C -5.89316 0.04334 0.46483
C -4.79285 0.87587 0.62878
C 0.20338 3.15898 -0.33994
O -0.38757 4.17363 -0.59846
H 0.98364 -0.56213 0.27504
H 3.92842 1.59688 -0.28840
H 2.42062 -2.37840 0.47257
H 4.74283 -3.26215 0.44478
H 6.24076 0.68498 -0.31328
H -2.34151 -1.13708 -0.57225
H -4.31857 -2.66847 -0.87823
H -6.89277 0.35365 0.74494
H -4.89696 1.87290 1.04437
C -2.35346 1.40725 0.45361
O -2.57957 2.51638 0.92897
N -6.84252 -2.11262 -0.25302
O -6.64502 -3.22079 -0.72603
O -7.94097 -1.69942 0.08344
N 6.96438 -1.85425 0.04772
O 7.12364 -3.05509 0.23347
O 7.88395 -1.07124 -0.14996

37
SCF Energy = -1398.17641327
Enthalpy 0K = -1397.924450
Enthalpy 298K = -1397.900579

Free Energy 298K = -1397.981569
Lowest Frequencies = 15.4986 cm-1
ASQ4c_d
C 3.68699 -2.44085 0.12054
C 2.38947 -1.93307 0.20453
C 2.16974 -0.57183 0.08384
C 3.26161 0.29495 -0.12224
C 4.56609 -0.23944 -0.20376
C 4.78033 -1.59857 -0.08403
N 3.10475 1.65377 -0.24682
C 1.98183 2.44137 -0.19838
C 2.03051 3.88339 -0.33641
O 2.94964 4.67127 -0.49026
C 0.58574 2.37491 -0.04124
N -0.29613 1.39497 0.07323
C -2.58097 0.66989 0.34182
C -3.84639 0.86772 0.90264
C -4.87608 -0.03401 0.66396
C -4.61394 -1.13569 -0.14569
C -3.36615 -1.36065 -0.71927
C -2.34933 -0.44504 -0.47027
C 0.49983 3.88113 -0.26136
O -0.38254 4.67981 -0.43107
H 3.94965 2.20176 -0.38505
H 5.40848 0.42873 -0.36242
H 1.16266 -0.16411 0.14455
H 1.56070 -2.61301 0.36606
H 5.77741 -2.01830 -0.14510
H -3.99664 1.74425 1.52447
H -5.86437 0.10035 1.08721
H -3.20940 -2.23219 -1.34367
H -1.36362 -0.57936 -0.90268
C -1.50152 1.69632 0.62796
O -1.76606 2.64510 1.36214
N 3.90858 -3.86944 0.24624
O 2.93741 -4.59219 0.42250
O 5.05929 -4.28416 0.16952
N -5.69482 -2.09556 -0.40489
O -6.78125 -1.88828 0.11266
O -5.45250 -3.05124 -1.12469

37
SCF Energy = -1398.17935579
Enthalpy 0K = -1397.927383
Enthalpy 298K = -1397.903661
Free Energy 298K = -1397.983680
Lowest Frequencies = 10.6161 cm-1
ASQ4c_e
C 0.63206 3.32932 -0.32012
C 1.65569 3.52720 0.60690
C 2.52914 2.49089 0.87490
C 2.39269 1.24953 0.22270
C 1.36745 1.08074 -0.73052
C 0.48480 2.11289 -0.98888
N 3.29926 0.24984 0.49086
C 3.22857 -1.06120 0.10646
C 4.34939 -1.96098 -0.13228
O 5.55625 -1.86586 -0.00319
C 2.24479 -2.03347 -0.16109
N 0.92406 -2.15458 -0.15445
C -1.24599 -1.33449 0.49319
C -2.01502 -0.43425 1.23685
C -3.39210 -0.36762 1.06119
C -3.97991 -1.22127 0.13217
C -3.24090 -2.12654 -0.62420
C -1.86363 -2.17447 -0.43973
C 3.31357 -3.01618 -0.55723
O 3.33244 -4.13048 -1.01734
H 4.18891 0.52602 0.89239
H 1.26746 0.13670 -1.25582
H 3.31533 2.61994 1.61339
H 1.74560 4.48286 1.10961
H -0.31444 1.99248 -1.71103
H -1.50706 0.20636 1.95068
H -4.00806 0.32504 1.62214
H -3.74407 -2.77086 -1.33524
H -1.24447 -2.86147 -1.00639
C 0.25044 -1.35773 0.71195
O 0.72811 -0.70173 1.64448
N -0.28422 4.41804 -0.60596
O -0.12913 5.47569 -0.00662
O -1.16586 4.23068 -1.43310
N -5.43580 -1.16737 -0.05496
O -5.93496 -1.91277 -0.88338
O -6.07292 -0.38214 0.62894

34
SCF Energy = -1011.35181941
Enthalpy 0K = -1011.113446
Enthalpy 298K = -1011.091203
Free Energy 298K = -1011.169817
Lowest Frequencies = 12.6382 cm-1
ASQ5_a
C 5.86685 -0.33135 0.78240

C 4.87198 -1.27351 0.53403
C 3.55216 -0.86390 0.36079
C 3.20906 0.49326 0.45116
C 4.21336 1.42661 0.72821
C 5.53296 1.01811 0.87565
N 1.86647 0.89094 0.30515
C 1.42488 2.05546 -0.18107
C 2.06724 3.25030 -0.86439
O 3.18074 3.56493 -1.17771
C 0.16363 2.61335 -0.34513
N -1.14832 2.29335 -0.09298
C -3.06978 1.02958 0.65878
C -3.73707 2.10606 1.25709
C -5.10541 2.05290 1.49955
C -5.82196 0.91754 1.13059
C -5.17381 -0.15749 0.52536
C -3.79913 -0.10988 0.29543
C 0.64865 3.82940 -0.99510
O 0.11459 4.81347 -1.44616
H -1.83263 2.95360 -0.44997
H 1.13242 0.24090 0.59070
H 3.95434 2.47450 0.82221
H 5.12093 -2.32705 0.46296
H 6.29852 1.76008 1.07768
H -3.16755 2.98039 1.56229
H -5.60503 2.89008 1.97563
H -5.73881 -1.03459 0.22867
C -1.58612 1.12026 0.47984
O -0.81471 0.24486 0.83025
H -6.89129 0.86224 1.30956
H 6.89497 -0.65575 0.90610
I 2.07887 -2.32331 -0.04617
I -2.92005 -1.76123 -0.68556

33
SCF Energy = -1010.82338740
Enthalpy 0K = -1010.599320
Enthalpy 298K = -1010.577367
Free Energy 298K = -1010.653242
Lowest Frequencies = 15.1570 cm-1
ASQ5b_b
C 2.89667 3.09255 0.51135
C 3.15255 1.86800 -0.09794
C 2.48309 0.71424 0.31636
C 1.50084 0.74730 1.33457
C 1.30040 2.00345 1.95619
C 1.97319 3.14564 1.55952
N 0.83832 -0.33167 1.87355
C 0.20536 -1.22752 1.18406
C -0.37796 -2.53571 1.69181
O -0.45273 -3.06298 2.77341
C -0.30583 -1.54851 -0.11167
N -0.30374 -1.04109 -1.40857
C -0.92935 1.32181 -0.98567
C -2.04823 1.32239 -0.14596
C -2.37187 2.46063 0.59763
C -1.60296 3.61385 0.47989
C -0.51680 3.64198 -0.39313
C -0.18921 2.50430 -1.11518
C -0.80817 -2.84469 0.25487
O -1.33257 -3.77110 -0.35124
H -0.21257 -1.74546 -2.13756
H 0.57487 2.03029 2.76411
H 3.89447 1.79776 -0.88787
H 1.76974 4.08888 2.06131
H -3.23878 2.44692 1.24987
H 0.08672 4.53876 -0.49529
H 0.65727 2.50219 -1.79520
C -0.52241 0.20516 -1.91115
O -0.38307 0.43761 -3.10715
H -1.86379 4.49180 1.06458
H 3.42910 3.98208 0.18693
I 3.15927 -1.12299 -0.49916
I -3.43339 -0.27816 -0.07705

33
SCF Energy = -1010.83920678
Enthalpy 0K = -1010.614631
Enthalpy 298K = -1010.592752
Free Energy 298K = -1010.670550
Lowest Frequencies = 9.6644 cm-1
ASQ5c_a
C -5.53214 -0.97054 0.72747
C -4.43250 -1.71036 0.30187
C -3.21722 -1.08355 0.03917
C -3.05804 0.31017 0.19770
C -4.18201 1.03899 0.63405
C -5.39159 0.40809 0.88639
N -1.83930 0.91893 -0.04065
C -1.53055 2.25003 -0.03189
C -2.26037 3.53695 -0.04383
O -3.41982 3.91424 -0.06364
C -0.26470 2.88662 -0.06216
N 1.03913 2.60558 -0.05574

C 2.95506 1.17704 -0.16049
C 3.76704 2.31026 -0.32853
C 5.15319 2.23144 -0.28059
C 5.76615 1.00282 -0.04069
C 4.98405 -0.13153 0.15396
C 3.59051 -0.04589 0.08833
C -0.90402 4.22693 -0.03174
O -0.51913 5.37479 -0.02225
H -1.01794 0.34245 -0.25782
H -4.10237 2.11490 0.73960
H -4.51386 -2.78443 0.16875
H -6.23481 1.00998 1.21344
H 3.26106 3.25534 -0.49412
H 5.75182 3.12634 -0.42458
H 5.45394 -1.08752 0.36064
C 1.45442 1.35025 -0.29698
O 0.77594 0.37454 -0.66461
H -6.47714 -1.46577 0.92816
H 6.84890 0.92166 0.00427
I -1.60373 -2.29479 -0.60438
I 2.55754 -1.85878 0.48982

33
SCF Energy = -1010.83573696
Enthalpy 0K = -1010.611189
Enthalpy 298K = -1010.589281
Free Energy 298K = -1010.668349
Lowest Frequencies = 4.8359 cm-1
ASQ5c_b
C -5.77225 0.84355 1.11094
C -5.13015 -0.37091 0.88791
C -3.82519 -0.40227 0.40247
C -3.11380 0.78417 0.12137
C -3.78144 2.00222 0.35906
C -5.08280 2.02527 0.83888
N -1.81160 0.74374 -0.34120
C -1.00040 1.78204 -0.70855
C -1.13648 3.22171 -1.02141
O -2.02656 4.05346 -1.07414
C 0.39072 1.78292 -0.97283
N 1.44343 0.96390 -0.94140
C 2.52228 -1.18003 -0.75871
C 3.64827 -0.84916 0.00447
C 4.76436 -1.69090 0.03279
C 4.77528 -2.87002 -0.70636
C 3.65620 -3.22559 -1.45750
C 2.54588 -2.39085 -1.46591
C 0.36685 3.23958 -1.26594
O 1.17693 4.08145 -1.57950
H -1.34678 -0.16231 -0.47233
H -3.27491 2.93294 0.12876
H -5.64214 -1.30605 1.09173
H -5.56114 2.98731 0.99995
H 5.62300 -1.42217 0.63942
H 3.64750 -4.14947 -2.02891
C 1.25436 -0.36074 -0.90436
O 0.19232 -0.99497 -1.06920
H -6.78974 0.86051 1.48903
H 5.65341 -3.50970 -0.68243
I -2.93829 -2.30315 0.11061
H 1.65176 -2.65110 -2.02389
I 3.75686 0.85600 1.25999

34
SCF Energy = -1011.35875905
Enthalpy 0K = -1011.120108
Enthalpy 298K = -1011.097835
Free Energy 298K = -1011.177364
Lowest Frequencies = 12.4726 cm-1
ASQ6_a
C -5.66813 -0.72210 -0.02572
C -4.59274 -1.60723 0.01346
C -3.29602 -1.10810 0.03814
C -3.06484 0.27219 0.02318
C -4.14548 1.15560 -0.01691
C -5.44423 0.65248 -0.04042
N -1.72031 0.68577 0.04617
C -1.18572 1.91231 0.06067
C -1.67502 3.35545 0.06638
O -2.73485 3.91689 0.05713
C 0.13574 2.34869 0.07780
N 1.40612 1.82561 0.07419
C 3.18543 0.16029 0.04646
C 4.15075 1.02833 -0.47282
C 5.49046 0.65174 -0.50613
C 5.86163 -0.59895 -0.01394
C 4.90749 -1.47912 0.49813
C 3.57103 -1.09731 0.51875
C -0.19748 3.76768 0.08314
O 0.45190 4.78564 0.09561
H 2.14389 2.52044 0.12668
H -1.01756 -0.05386 0.07784
H -3.98797 2.22815 -0.02755
H -2.45577 -1.79730 0.06875

H -4.75717 -2.67934 0.02498
H -6.27815 1.34578 -0.07069
H 3.87691 1.99198 -0.89395
H 6.23326 1.32523 -0.91951
H 5.20195 -2.45268 0.87499
H 2.80999 -1.76903 0.90285
C 1.73234 0.49048 0.10325
O 0.87237 -0.37684 0.18489
I 7.88815 -1.17174 -0.05682
I -7.64054 -1.46862 -0.06447

33
SCF Energy = -1010.84327446
Enthalpy 0K = -1010.618588
Enthalpy 298K = -1010.596879
Free Energy 298K = -1010.672269
Lowest Frequencies = 19.2860 cm-1
ASQ6_b
C -1.23887 -1.98976 -0.73256
C -0.04283 -2.59750 -0.36292
C 1.16525 -1.99978 -0.71315
C 1.20275 -0.78204 -1.42642
C -0.02903 -0.22523 -1.82836
C -1.23785 -0.80925 -1.47815
N 2.37045 -0.14975 -1.80643
C 3.42387 -0.22028 -1.04763
C 4.86254 0.13376 -1.37287
O 5.42857 0.58691 -2.33642
C 3.83813 -0.51681 0.29138
N 3.29265 -0.95502 1.48980
C 1.13347 0.26292 1.53438
C 1.57685 1.43544 0.91852
C 0.66009 2.38782 0.47655
C -0.69877 2.15224 0.65827
C -1.16015 1.00642 1.30345
C -0.23454 0.07075 1.74872
C 5.24224 -0.31317 0.04500
O 6.26279 -0.46041 0.70563
H 3.92659 -1.50145 2.06911
H -0.00872 0.70070 -2.39669
H 2.09876 -2.48197 -0.43578
H -0.04301 -3.52063 0.20894
H -2.17233 -0.33545 -1.76559
H 2.63680 1.61428 0.76999
H 1.00892 3.28654 -0.02051
H -2.22290 0.82899 1.43439
H -0.56367 -0.83569 2.24782
C 2.05698 -0.79105 2.06678
O 1.74013 -1.46662 3.03996
I -2.10384 3.53953 -0.10483
I -3.08248 -2.83251 -0.11506

33
SCF Energy = -1010.85401209
Enthalpy 0K = -1010.629086
Enthalpy 298K = -1010.608089
Free Energy 298K = -1010.682814
Lowest Frequencies = -3.3875 cm-1
ASQ6c_a
C 5.58980 -0.72174 -0.00034
C 5.37786 0.65492 -0.00233
C 4.08415 1.16858 -0.00117
C 2.98275 0.29767 0.00202
C 3.21541 -1.09004 0.00405
C 4.50750 -1.59920 0.00285
N 1.66700 0.72262 0.00316
C 1.14354 1.97756 0.00183
C 1.64305 3.37012 0.00016
O 2.72356 3.93497 -0.00056
C -0.21216 2.38729 0.00151
N -1.45290 1.88719 0.00171
C -3.12179 0.17613 0.00377
C -4.13360 1.14003 -0.00238
C -5.47478 0.76119 -0.00426
C -5.79408 -0.59506 0.00021
C -4.80334 -1.57378 0.00657
C -3.46734 -1.17672 0.00824
C 0.18677 3.81703 -0.00041
O -0.38783 4.88265 -0.00182
H 0.92285 0.01307 0.00593
H 2.36728 -1.77011 0.00653
H 3.92713 2.24356 -0.00256
H 6.21844 1.34173 -0.00477
H 4.66355 -2.67320 0.00439
H -3.84810 2.18692 -0.00567
H -6.25710 1.51313 -0.00915
H -5.06519 -2.62698 0.01017
H -2.66861 -1.91190 0.01305
C -1.66115 0.56190 0.00549
O -0.82319 -0.36760 0.01043
I 7.56372 -1.48862 -0.00227
I -7.83230 -1.18158 -0.00284

34

SCF Energy = -2828.07421355
Enthalpy 0K = -2827.852776
Enthalpy 298K = -2827.828986
Free Energy 298K = -2827.909957
Lowest Frequencies = 13.8793 cm-1
ASQ7_a
C -5.65613 -0.83712 -0.07668
C -4.55100 -1.69082 -0.09313
C -3.26388 -1.16681 -0.06058
C -3.06515 0.21525 -0.01222
C -4.16531 1.07610 0.00248
C -5.44606 0.53944 -0.02858
N -1.73002 0.65425 0.01333
C -1.22498 1.89185 0.09459
C -1.75032 3.31887 0.20135
O -2.82357 3.85144 0.24734
C 0.08458 2.35974 0.11502
N 1.36750 1.87174 0.05450
C 3.18560 0.25914 -0.11298
C 4.12187 1.18374 -0.58544
C 5.46343 0.83364 -0.66023
C 5.88283 -0.43564 -0.26307
C 4.94482 -1.36660 0.20010
C 3.60099 -1.01712 0.26599
C -0.28286 3.76746 0.21682
O 0.34196 4.79784 0.28202
H 2.08849 2.58106 0.13846
H -1.01012 -0.06897 -0.01254
H -4.03439 2.15103 0.04218
H -2.41788 -1.84776 -0.07276
H -6.30661 1.19997 -0.01603
H 3.82357 2.16742 -0.93576
H 6.19911 1.53729 -1.03412
H 2.86779 -1.73720 0.61405
C 1.72508 0.54668 -0.00735
O 0.88997 -0.34626 0.03483
Cl -7.27406 -1.45159 -0.11327
Cl 7.55940 -0.83166 -0.36273
Cl -4.74423 -3.41052 -0.15238
Cl 5.42594 -2.95068 0.69377

34
SCF Energy = -2828.07335837
Enthalpy 0K = -2827.852008
Enthalpy 298K = -2827.829130
Free Energy 298K = -2827.906432
Lowest Frequencies = -2.2135 cm-1
ASQ7_b
C -5.60317 -1.52816 0.16089
C -5.38576 -0.15009 0.09506
C -4.09468 0.36859 0.02142
C -3.00581 -0.50175 0.01270
C -3.21728 -1.88414 0.07970
C -4.50628 -2.38788 0.15317
N -1.67017 -0.07000 -0.05837
C -1.15607 1.16301 -0.15424
C -1.67421 2.59443 -0.22824
O -2.74491 3.13315 -0.22392
C 0.15499 1.61977 -0.22758
N 1.43536 1.11975 -0.22700
C 3.24157 -0.51731 -0.16067
C 3.63606 -1.78804 -0.58771
C 4.97830 -2.13607 -0.58349
C 5.93955 -1.22663 -0.13967
C 5.54644 0.03952 0.30685
C 4.19877 0.39003 0.29438
C -0.20461 3.03182 -0.30519
O 0.42524 4.05701 -0.39224
H 2.15828 1.82328 -0.34029
H -0.95741 -0.80041 -0.06516
H -2.37088 -2.56524 0.07408
H -3.96199 1.44362 -0.03063
H -4.67447 -3.45825 0.20480
H 2.88038 -2.49083 -0.92171
H 5.29970 -3.11516 -0.92192
H 3.92791 1.36698 0.68366
C 1.78177 -0.20875 -0.19312
O 0.93680 -1.09379 -0.20414
Cl -7.19942 -2.19248 0.24928
Cl 7.60081 -1.69290 -0.14499
Cl -6.71387 0.95960 0.10237
Cl 6.70233 1.18499 0.88813

34
SCF Energy = -2828.07362377
Enthalpy 0K = -2827.852341
Enthalpy 298K = -2827.828507
Free Energy 298K = -2827.910486
Lowest Frequencies = 6.3685 cm-1
ASQ7_c
C 5.34834 -1.77323 -0.12528
C 5.28562 -0.38037 -0.04345
C 4.05941 0.27978 0.00268
C 2.87990 -0.46215 -0.03242

C 2.93622 -1.85873 -0.11300
C 4.16198 -2.50366 -0.15928
N 1.59966 0.11696 0.00473
C 1.22475 1.39905 0.09777
C 1.89712 2.76214 0.21198
O 3.02092 3.17656 0.25634
C -0.02853 2.00045 0.12744
N -1.35587 1.64917 0.06890
C -3.33204 0.23549 -0.10880
C -4.16994 1.25661 -0.56705
C -5.54026 1.04573 -0.64338
C -6.08637 -0.17960 -0.26252
C -5.24741 -1.20691 0.18664
C -3.87512 -0.99650 0.25476
C 0.48408 3.36164 0.23767
O -0.03030 4.45060 0.31300
H -1.99854 2.42918 0.16098
H 0.80932 -0.52810 -0.02598
H 2.01888 -2.44013 -0.14040
H 4.04708 1.36223 0.06753
H 4.21016 -3.58540 -0.22271
H -3.77375 2.20947 -0.90533
H -6.20082 1.82556 -1.00629
H -3.21879 -1.79169 0.59242
C -1.84925 0.36965 -0.00475
O -1.11148 -0.60604 0.02538
Cl 6.86135 -2.61208 -0.18810
Cl -7.79432 -0.40254 -0.36464
Cl 6.72932 0.57293 0.00260
Cl -5.88602 -2.74120 0.65911

34
SCF Energy = -2828.06314744
Enthalpy 0K = -2827.842489
Enthalpy 298K = -2827.818827
Free Energy 298K = -2827.896943
Lowest Frequencies = 20.1537 cm-1
ASQ7_d
C 3.27964 0.50458 -0.92097
C 2.49587 1.13702 0.04698
C 1.11127 1.19375 -0.09309
C 0.50701 0.62458 -1.21090
C 1.28639 -0.00117 -2.18724
C 2.66376 -0.06128 -2.03635
N -0.89915 0.57983 -1.34421
C -1.77595 1.35648 -0.67500
C -1.72160 2.79235 -0.22185
O -0.88278 3.64672 -0.19993
C -3.08604 1.21434 -0.24414
N -4.05540 0.24466 -0.20673
C -2.52900 -1.65632 -0.03085
C -1.97213 -2.56915 -0.92850
C -0.63900 -2.94407 -0.78953
C 0.12809 -2.43811 0.26113
C -0.45908 -1.59156 1.21021
C -1.78339 -1.19494 1.05325
C -3.20239 2.62217 0.19302
O -4.09798 3.29660 0.62530
H -5.01924 0.57048 -0.16837
H -1.25761 -0.28334 -1.73814
H 0.81311 -0.43849 -3.06190
H 0.52350 1.66487 0.68710
H 3.27806 -0.55006 -2.78488
H -2.57609 -2.95828 -1.74309
H -0.17474 -3.62264 -1.49762
H -2.21605 -0.50557 1.77286
C -3.91102 -1.14089 -0.28221
O -4.85646 -1.85383 -0.53452
Cl 4.99840 0.39229 -0.75842
Cl 1.80000 -2.85027 0.35746
Cl 3.20644 1.82731 1.46307
Cl 0.44541 -0.98410 2.54966

34
SCF Energy = -2828.06384899
Enthalpy 0K = -2827.842980
Enthalpy 298K = -2827.819248
Free Energy 298K = -2827.898693
Lowest Frequencies = 12.2079 cm-1
ASQ7_e
C 3.18786 1.49062 -0.01652
C 2.80912 0.49615 -0.92109
C 1.46582 0.30447 -1.22332
C 0.48606 1.09416 -0.61887
C 0.85678 2.08808 0.28918
C 2.20278 2.28041 0.57258
N -0.85700 0.79192 -0.92296
C -1.96660 1.40720 -0.45872
C -2.29624 2.83304 -0.08313
O -1.68733 3.86044 0.01859
C -3.28264 1.00545 -0.26443
N -4.07509 -0.10539 -0.36918
C -2.34088 -1.83546 -0.17333
C -1.65341 -2.69598 -1.03301

C -0.32278 -3.00601 -0.77733
C 0.32027 -2.47776 0.34446
C -0.38618 -1.65723 1.23250
C -1.71726 -1.34295 0.97224
C -3.75149 2.35945 0.08609
O -4.82927 2.83253 0.33132
H -5.07471 0.08170 -0.43615
H -0.99458 -0.12804 -1.32784
H 0.11558 2.71758 0.76499
H 1.19179 -0.47286 -1.93191
H 2.50075 3.05175 1.27470
H -2.16180 -3.10245 -1.90196
H 0.23705 -3.65134 -1.44621
H -2.24642 -0.68697 1.65777
C -3.74124 -1.45091 -0.52333
O -4.56455 -2.24588 -0.91975
Cl 4.84890 1.75934 0.38606
Cl 1.98899 -2.82944 0.59450
Cl 3.98193 -0.51984 -1.68666
Cl 0.37937 -0.97172 2.61941

34
SCF Energy = -2828.06374495
Enthalpy 0K = -2827.842979
Enthalpy 298K = -2827.819252
Free Energy 298K = -2827.898424
Lowest Frequencies = 12.7787 cm-1
ASQ7_f
C -2.99612 -1.78686 0.06196
C -2.69477 -0.72104 -0.78969
C -1.37163 -0.43315 -1.10307
C -0.33589 -1.19137 -0.55326
C -0.62811 -2.25821 0.29857
C -1.95572 -2.54939 0.58850
N 0.97976 -0.78061 -0.84476
C 2.13760 -1.35064 -0.45089
C 2.58146 -2.76695 -0.17319
O 2.04836 -3.83775 -0.09416
C 3.42643 -0.86447 -0.26924
N 4.09538 0.33064 -0.31903
C 2.21538 1.75299 0.33003
C 1.84706 1.07999 1.49766
C 0.53411 1.13960 1.94364
C -0.42400 1.84792 1.21606
C -0.04601 2.55317 0.06688
C 1.28096 2.52218 -0.36130
C 4.00851 -2.19892 -0.03439
O 5.12423 -2.61315 0.13583
H 5.09625 0.27463 -0.49890
H 1.04830 0.17442 -1.17878
H 0.16048 -2.86911 0.72096
H -1.15903 0.39942 -1.76925
H -2.19498 -3.37861 1.24581
H 2.57984 0.49712 2.04843
H 0.22669 0.61437 2.84178
H 1.57732 3.07411 -1.24881
C 3.59404 1.63058 -0.23673
O 4.25645 2.57608 -0.60068
Cl -4.63046 -2.17179 0.48115
Cl -2.06595 1.81340 1.74013
Cl -3.93912 0.27437 -1.46107
Cl -1.20758 3.43281 -0.86207

34
SCF Energy = -2828.06269274
Enthalpy 0K = -2827.842132
Enthalpy 298K = -2827.818365
Free Energy 298K = -2827.898031
Lowest Frequencies = 11.0076 cm-1
ASQ7_g
C 3.33623 -0.52342 -0.63711
C 2.59771 -1.49000 0.04950
C 1.21314 -1.56243 -0.09340
C 0.56393 -0.66948 -0.94268
C 1.29866 0.29506 -1.64006
C 2.67363 0.36673 -1.48096
N -0.83864 -0.64151 -1.07371
C -1.73045 -1.52774 -0.58486
C -1.70918 -3.01895 -0.35760
O -0.88188 -3.88350 -0.41683
C -3.06642 -1.44233 -0.21848
N -4.03711 -0.48136 -0.09916
C -2.53544 1.36122 0.46845
C -1.86291 0.75032 1.52992
C -0.56505 1.13315 1.83714
C 0.07943 2.10802 1.07331
C -0.60777 2.74570 0.03386
C -1.92506 2.38625 -0.25150
C -3.21014 -2.89707 -0.01192
O -4.12930 -3.62315 0.25719
H -5.00056 -0.80231 -0.17386
H -1.20906 0.26173 -1.34723
H 0.79310 0.99577 -2.30000
H 0.66711 -2.32075 0.45554

H 3.24747 1.12131 -2.00835
H -2.34571 -0.03448 2.10523
H -0.02290 0.66192 2.65036
H -2.46216 2.88617 -1.05263
C -3.89308 0.89980 0.04099
O -4.82153 1.64750 -0.16914
Cl 5.05176 -0.39536 -0.45268
Cl 1.72473 2.48758 1.42265
Cl 3.37049 -2.60955 1.11807
Cl 0.15780 3.95703 -0.93370

34
SCF Energy = -2828.07421355
Enthalpy 0K = -2827.852776
Enthalpy 298K = -2827.828986
Free Energy 298K = -2827.909957
Lowest Frequencies = 13.8782 cm-1
ASQ7_dd
C -5.65611 -0.83714 -0.07667
C -4.55098 -1.69082 -0.09313
C -3.26387 -1.16681 -0.06059
C -3.06515 0.21526 -0.01222
C -4.16531 1.07609 0.00249
C -5.44606 0.53943 -0.02857
N -1.73002 0.65427 0.01332
C -1.22498 1.89186 0.09459
C -1.75033 3.31888 0.20135
O -2.82357 3.85145 0.24733
C 0.08458 2.35976 0.11502
N 1.36750 1.87176 0.05450
C 3.18559 0.25915 -0.11297
C 4.12188 1.18374 -0.58543
C 5.46343 0.83364 -0.66022
C 5.88282 -0.43564 -0.26306
C 4.94481 -1.36660 0.20010
C 3.60097 -1.01711 0.26599
C -0.28287 3.76747 0.21682
O 0.34195 4.79785 0.28202
H 2.08849 2.58108 0.13845
H -1.01012 -0.06896 -0.01256
H -4.03440 2.15102 0.04219
H -2.41786 -1.84775 -0.07278
H -6.30662 1.19995 -0.01601
H 3.82359 2.16743 -0.93575
H 6.19912 1.53728 -1.03411
H 2.86777 -1.73718 0.61404
C 1.72508 0.54670 -0.00735
O 0.88996 -0.34624 0.03484
Cl -7.27405 -1.45162 -0.11325
Cl 7.55939 -0.83168 -0.36273
Cl -4.74420 -3.41053 -0.15239
Cl 5.42591 -2.95069 0.69376

34
SCF Energy = -2828.07400212
Enthalpy 0K = -2827.852543
Enthalpy 298K = -2827.828745
Free Energy 298K = -2827.910040
Lowest Frequencies = 8.5873 cm-1
ASQ7_du
C -5.83941 -0.52604 -0.16517
C -4.84372 -1.50250 -0.09259
C -3.50676 -1.13131 -0.00890
C -3.14819 0.21901 0.00224
C -4.13816 1.20198 -0.07129
C -5.47040 0.81750 -0.15243
N -1.77330 0.50011 0.08114
C -1.12993 1.67253 0.15557
C -1.48927 3.15278 0.20780
O -2.49427 3.80655 0.19490
C 0.22327 1.98577 0.22364
N 1.44167 1.35025 0.23025
C 3.05985 -0.47314 0.18741
C 3.32209 -1.76663 0.64655
C 4.61958 -2.25585 0.63831
C 5.66608 -1.46688 0.15803
C 5.40417 -0.17883 -0.32087
C 4.10188 0.31398 -0.30382
C 0.01859 3.42927 0.27923
O 0.75520 4.38199 0.35190
H 2.23718 1.97307 0.32860
H -1.14342 -0.30246 0.10937
H -3.88295 2.25502 -0.06067
H -2.74778 -1.90612 0.04783
H -6.24615 1.57387 -0.20875
H 2.50046 -2.37549 1.00827
H 4.83939 -3.25399 1.00142
H 3.93051 1.30286 -0.71855
C 1.64223 -0.00894 0.22388
O 0.70685 -0.79659 0.26083
Cl -7.51473 -0.94908 -0.27063
Cl 7.26841 -2.10790 0.15916
Cl -5.23623 -3.18910 -0.10366
Cl 6.66728 0.81955 -0.94922

34
SCF Energy = -2828.07362377
Enthalpy 0K = -2827.852341
Enthalpy 298K = -2827.828507
Free Energy 298K = -2827.910486
Lowest Frequencies = 6.3714 cm-1
ASQ7_ud
C 5.34834 -1.77323 -0.12528
C 5.28562 -0.38037 -0.04345
C 4.05941 0.27978 0.00268
C 2.87990 -0.46215 -0.03242
C 2.93622 -1.85873 -0.11300
C 4.16198 -2.50366 -0.15928
N 1.59966 0.11696 0.00473
C 1.22475 1.39905 0.09777
C 1.89712 2.76214 0.21198
O 3.02092 3.17656 0.25634
C -0.02853 2.00045 0.12744
N -1.35587 1.64917 0.06890
C -3.33204 0.23549 -0.10880
C -4.16994 1.25661 -0.56705
C -5.54026 1.04573 -0.64338
C -6.08637 -0.17960 -0.26252
C -5.24741 -1.20691 0.18664
C -3.87512 -0.99650 0.25476
C 0.48408 3.36164 0.23767
O -0.03030 4.45060 0.31300
H -1.99854 2.42918 0.16098
H 0.80932 -0.52810 -0.02598
H 2.01888 -2.44013 -0.14040
H 4.04708 1.36223 0.06753
H 4.21016 -3.58540 -0.22271
H -3.77375 2.20947 -0.90533
H -6.20082 1.82556 -1.00629
H -3.21879 -1.79169 0.59242
C -1.84925 0.36965 -0.00475
O -1.11148 -0.60604 0.02538
Cl 6.86135 -2.61208 -0.18810
Cl -7.79432 -0.40254 -0.36464
Cl 6.72932 0.57293 0.00260
Cl -5.88602 -2.74120 0.65911

34
SCF Energy = -2828.07335837
Enthalpy 0K = -2827.852008
Enthalpy 298K = -2827.829130
Free Energy 298K = -2827.906432
Lowest Frequencies = -2.2132 cm-1
ASQ7_uu
C -5.60317 -1.52816 0.16089
C -5.38576 -0.15009 0.09506
C -4.09468 0.36859 0.02142
C -3.00581 -0.50175 0.01270
C -3.21728 -1.88414 0.07970
C -4.50628 -2.38788 0.15317
N -1.67017 -0.07000 -0.05837
C -1.15607 1.16301 -0.15424
C -1.67421 2.59443 -0.22824
O -2.74491 3.13315 -0.22392
C 0.15499 1.61977 -0.22758
N 1.43536 1.11975 -0.22700
C 3.24157 -0.51731 -0.16067
C 3.63606 -1.78804 -0.58771
C 4.97830 -2.13607 -0.58349
C 5.93955 -1.22663 -0.13967
C 5.54644 0.03952 0.30685
C 4.19877 0.39003 0.29438
C -0.20461 3.03182 -0.30519
O 0.42524 4.05701 -0.39224
H 2.15828 1.82328 -0.34029
H -0.95741 -0.80041 -0.06516
H -2.37088 -2.56524 0.07408
H -3.96199 1.44362 -0.03063
H -4.67447 -3.45825 0.20480
H 2.88038 -2.49083 -0.92171
H 5.29970 -3.11516 -0.92192
H 3.92791 1.36698 0.68366
C 1.78177 -0.20875 -0.19312
O 0.93680 -1.09379 -0.20414
Cl -7.19942 -2.19248 0.24928
Cl 7.60081 -1.69290 -0.14499
Cl -6.71387 0.95960 0.10237
Cl 6.70233 1.18499 0.88813

33
SCF Energy = -2827.56658271
Enthalpy 0K = -2827.359070
Enthalpy 298K = -2827.335798
Free Energy 298K = -2827.412312
Lowest Frequencies = 28.7594 cm-1
ASQ7b_b
C -1.59888 -2.16331 -0.23150
C -0.35911 -2.56721 0.25920

C 0.81442 -2.00184 -0.22187
C 0.78338 -0.99775 -1.21398
C -0.47424 -0.63446 -1.73259
C -1.64202 -1.19884 -1.24427
N 1.90828 -0.40358 -1.74862
C 2.95448 -0.21256 -0.99910
C 4.37248 0.14280 -1.40412
O 4.92411 0.37311 -2.45076
C 3.36214 -0.13300 0.37011
N 2.82149 -0.28984 1.63819
C 0.58286 0.74086 1.36290
C 0.95179 1.74401 0.46349
C -0.02732 2.49083 -0.18089
C -1.37579 2.24751 0.06882
C -1.74651 1.26927 0.99656
C -0.76747 0.52574 1.64137
C 4.75530 0.09683 0.08206
O 5.76988 0.19186 0.75940
H 3.47633 -0.62855 2.34005
H -0.51865 0.12110 -2.51045
H 1.77127 -2.34155 0.16354
H -0.32424 -3.32467 1.03653
H 1.99676 1.94676 0.25634
H 0.24700 3.26017 -0.89467
H -1.04814 -0.23571 2.36190
C 1.56288 -0.08206 2.14598
O 1.26700 -0.51733 3.25302
Cl -2.56974 3.18286 -0.77598
Cl -3.04932 -2.87925 0.41479
Cl -3.41289 0.95472 1.36176
Cl -3.16141 -0.66571 -1.90918

33
SCF Energy = -2827.57628057
Enthalpy 0K = -2827.368620
Enthalpy 298K = -2827.346047
Free Energy 298K = -2827.422663
Lowest Frequencies = -5.7610 cm-1
ASQ7c_a
C 5.56658 -0.86008 -0.00001
C 4.44838 -1.69449 -0.00000
C 3.16771 -1.15908 -0.00000
C 2.97434 0.23250 -0.00001
C 4.09906 1.07421 -0.00001
C 5.37110 0.52016 -0.00001
N 1.67146 0.69166 -0.00001
C 1.18710 1.96332 -0.00000
C 1.73013 3.34015 0.00000
O 2.82716 3.87107 -0.00000
C -0.15433 2.41470 0.00001
N -1.41013 1.95322 0.00001
C -3.12942 0.29713 0.00001
C -4.11325 1.28965 -0.00001
C -5.45806 0.93993 -0.00002
C -5.83349 -0.40318 -0.00001
C -4.85297 -1.39691 0.00000
C -3.50706 -1.04445 0.00001
C 0.28783 3.83192 0.00001
O -0.25396 4.91385 0.00002
H 0.90620 0.00468 -0.00000
H 3.97326 2.15284 -0.00002
H 2.31164 -1.82707 0.00000
H 6.24016 1.17060 -0.00002
H -3.80078 2.32816 -0.00001
H -6.23217 1.70053 -0.00003
H -2.73593 -1.80776 0.00002
C -1.65650 0.63540 0.00001
O -0.84971 -0.32022 0.00003
Cl 7.18659 -1.49852 -0.00001
Cl -7.52681 -0.80490 -0.00002
Cl 4.62316 -3.42697 0.00001
Cl -5.28544 -3.08368 0.00001

33
SCF Energy = -2827.57628057
Enthalpy 0K = -2827.368620
Enthalpy 298K = -2827.346047
Free Energy 298K = -2827.422663
Lowest Frequencies = -5.7602 cm-1
ASQ7c_dd
C -5.56658 -0.86008 -0.00000
C -4.44838 -1.69449 0.00000
C -3.16771 -1.15908 0.00000
C -2.97434 0.23250 0.00000
C -4.09906 1.07421 -0.00000
C -5.37110 0.52016 -0.00000
N -1.67146 0.69166 0.00000
C -1.18710 1.96332 0.00000
C -1.73013 3.34015 0.00000
O -2.82716 3.87107 0.00000
C 0.15433 2.41470 0.00000
N 1.41013 1.95322 0.00000
C 3.12942 0.29713 0.00000
C 4.11325 1.28965 -0.00000

C 5.45805 0.93993 -0.00000
C 5.83349 -0.40318 -0.00000
C 4.85297 -1.39691 0.00000
C 3.50706 -1.04445 0.00000
C -0.28782 3.83192 0.00000
O 0.25396 4.91385 0.00000
H -0.90620 0.00468 0.00000
H -3.97326 2.15284 -0.00000
H -2.31164 -1.82707 0.00000
H -6.24016 1.17061 -0.00001
H 3.80078 2.32816 -0.00000
H 6.23217 1.70053 -0.00000
H 2.73593 -1.80776 0.00000
C 1.65650 0.63540 0.00000
O 0.84971 -0.32022 0.00000
Cl -7.18659 -1.49852 -0.00000
Cl 7.52681 -0.80490 -0.00000
Cl -4.62316 -3.42697 0.00000
Cl 5.28544 -3.08368 0.00000

33
SCF Energy = -2827.57576176
Enthalpy 0K = -2827.368092
Enthalpy 298K = -2827.344596
Free Energy 298K = -2827.425388
Lowest Frequencies = 5.9360 cm-1
ASQ7c_du
C -5.78020 -0.51909 -0.00000
C -4.77682 -1.48832 0.00000
C -3.43864 -1.11992 0.00000
C -3.07001 0.23593 -0.00000
C -4.07907 1.21345 -0.00001
C -5.41106 0.82525 -0.00001
N -1.71968 0.52547 -0.00000
C -1.07632 1.72496 -0.00000
C -1.43977 3.15930 -0.00000
O -2.46065 3.82500 -0.00001
C 0.31169 2.00125 0.00000
N 1.49809 1.38229 0.00000
C 2.98709 -0.48800 -0.00000
C 3.19466 -1.86866 -0.00001
C 4.48406 -2.38680 -0.00001
C 5.58015 -1.52609 -0.00000
C 5.37747 -0.14360 0.00000
C 4.08518 0.37254 0.00000
C 0.05358 3.46388 0.00000
O 0.72781 4.46814 0.00001
H -1.04805 -0.25330 -0.00001
H -3.81723 2.26736 -0.00001
H -2.67414 -1.89104 0.00001
H -6.19053 1.58076 -0.00001
H 2.32807 -2.52136 -0.00001
H 4.65774 -3.45810 -0.00001
H 3.91452 1.44396 0.00001
C 1.57258 0.04410 -0.00000
O 0.64893 -0.79966 -0.00001
Cl -7.46791 -0.94726 -0.00000
Cl 7.18294 -2.20502 -0.00000
Cl -5.17011 -3.18497 0.00001
Cl 6.72595 0.95657 0.00001

33
SCF Energy = -2827.57550441
Enthalpy 0K = -2827.367890
Enthalpy 298K = -2827.345309
Free Energy 298K = -2827.421883
Lowest Frequencies = -2.4578 cm-1
ASQ7c_ud
C 5.24632 -1.79439 0.00000
C 5.20193 -0.39941 0.00004
C 3.99236 0.28755 0.00001
C 2.78768 -0.42998 -0.00006
C 2.83269 -1.83675 -0.00010
C 4.04611 -2.50339 -0.00007
N 1.54170 0.16632 -0.00009
C 1.18909 1.47996 -0.00006
C 1.87299 2.79192 -0.00005
O 3.02034 3.20083 -0.00005
C -0.09762 2.06721 -0.00004
N -1.39471 1.73631 -0.00003
C -3.27439 0.26615 -0.00003
C -4.15025 1.35523 0.00003
C -5.52399 1.14687 0.00007
C -6.03694 -0.15006 0.00006
C -5.16453 -1.24000 -0.00000
C -3.78931 -1.02900 -0.00004
C 0.48865 3.43160 -0.00003
O 0.06116 4.56339 -0.00001
H 0.71043 -0.43914 -0.00012
H 1.90350 -2.39960 -0.00016
H 3.98990 1.37463 0.00004
H 4.07500 -3.58827 -0.00011
H -3.73147 2.35566 0.00004
H -6.21507 1.98360 0.00012

H -3.10162 -1.86821 -0.00009
C -1.77434 0.45120 -0.00007
O -1.07007 -0.58300 -0.00014
Cl 6.75199 -2.66942 0.00005
Cl -7.76282 -0.37373 0.00011
Cl 6.67265 0.53078 0.00014
Cl -5.76946 -2.87322 -0.00002

33
SCF Energy = -2827.57488021
Enthalpy 0K = -2827.367256
Enthalpy 298K = -2827.343777
Free Energy 298K = -2827.424325
Lowest Frequencies = 5.9433 cm-1
ASQ7c_uu
C -5.53179 -1.53209 0.02312
C -5.31886 -0.15268 0.02382
C -4.03524 0.38313 0.00630
C -2.92620 -0.47495 -0.01283
C -3.14142 -1.86607 -0.01393
C -4.42638 -2.38125 0.00411
N -1.61745 -0.03443 -0.02970
C -1.10717 1.22674 -0.03340
C -1.62723 2.61161 -0.03335
O -2.71676 3.15614 -0.03140
C 0.24124 1.65338 -0.03740
N 1.48849 1.16666 -0.03501
C 3.17130 -0.53062 -0.03961
C 3.52816 -1.87999 -0.07354
C 4.86593 -2.25526 -0.05529
C 5.86145 -1.28162 -0.00104
C 5.50938 0.07010 0.03383
C 4.16894 0.44314 0.01352
C -0.17540 3.07920 -0.03550
O 0.38537 4.15080 -0.03565
H -0.86607 -0.73617 -0.05003
H -2.28711 -2.53703 -0.02867
H -3.90120 1.46197 0.00539
H -4.58627 -3.45475 0.00349
H 2.73801 -2.62223 -0.11429
H 5.15545 -3.30086 -0.08177
H 3.88241 1.48928 0.03906
C 1.70744 -0.15471 -0.05833
O 0.88115 -1.09401 -0.09609
Cl -7.13249 -2.21836 0.04436
Cl 7.52772 -1.78363 0.02254
Cl -6.66695 0.94740 0.04559
Cl 6.72964 1.30885 0.10645

34
SCF Energy = -1908.95026673
Enthalpy 0K = -1908.709443
Enthalpy 298K = -1908.688099
Free Energy 298K = -1908.762660
Lowest Frequencies = 16.1585 cm-1
ASQ8_a
C 5.58488 -1.38575 0.07086
C 4.49397 -2.24952 0.05251
C 3.20922 -1.72242 0.02329
C 3.00917 -0.33714 0.01283
C 4.10935 0.52299 0.03280
C 5.39592 -0.00775 0.06133
N 1.67352 0.10660 -0.01500
C 1.16724 1.34422 -0.05075
C 1.68929 2.77567 -0.07949
O 2.76176 3.31281 -0.07817
C -0.14390 1.81094 -0.07643
N -1.42615 1.31751 -0.06564
C -3.24345 -0.30475 -0.01474
C -4.18816 0.59351 0.49204
C -5.53564 0.25105 0.52727
C -5.93179 -0.99581 0.04926
C -5.00288 -1.90785 -0.44885
C -3.65866 -1.55923 -0.47139
C 0.22173 3.22131 -0.10461
O -0.40416 4.25367 -0.13432
H -2.14731 2.02846 -0.13112
H 0.95425 -0.61735 -0.03495
H 3.97494 1.59857 0.02404
H 2.35364 -2.39276 0.00858
H 4.64825 -3.32321 0.06049
H 6.25382 0.65618 0.07587
H -3.89065 1.55506 0.90128
H -6.27295 0.93773 0.92848
H -5.33431 -2.87535 -0.81007
H -2.91311 -2.25368 -0.84479
C -1.78332 -0.00990 -0.07456
O -0.94358 -0.89813 -0.14206
Cl 7.19971 -2.03787 0.10459
Cl -7.61313 -1.42488 0.08451

33
SCF Energy = -1908.43323758
Enthalpy 0K = -1908.206495

Enthalpy 298K = -1908.185655
Free Energy 298K = -1908.256485
Lowest Frequencies = 32.1992 cm-1
ASQ8b_b
C -2.24315 -1.97697 -0.68640
C -1.04876 -2.51637 -0.22486
C 0.15578 -1.91910 -0.58671
C 0.18807 -0.76971 -1.40503
C -1.04207 -0.28284 -1.89246
C -2.24670 -0.86876 -1.53208
N 1.35447 -0.14407 -1.80708
C 2.38184 -0.11623 -1.01220
C 3.82142 0.24996 -1.32038
O 4.40837 0.63527 -2.30107
C 2.75882 -0.28374 0.36072
N 2.18064 -0.63098 1.57395
C 0.00163 0.54280 1.44052
C 0.44828 1.66944 0.74554
C -0.46646 2.56850 0.20282
C -1.82543 2.32589 0.36174
C -2.29262 1.22664 1.07671
C -1.37048 0.34355 1.62228
C 4.16382 -0.06085 0.14255
O 5.16583 -0.11855 0.84506
H 2.80237 -1.11476 2.21831
H -1.02375 0.58948 -2.53968
H 1.09079 -2.34830 -0.23744
H -1.05891 -3.38639 0.42502
H -3.18884 -0.45952 -1.88562
H 1.50988 1.85302 0.61738
H -0.12702 3.43571 -0.35324
H -3.35921 1.05450 1.18011
H -1.70230 -0.52691 2.17960
C 0.92187 -0.44529 2.09078
O 0.58075 -1.04474 3.10520
Cl -2.98037 3.42161 -0.36561
Cl -3.77042 -2.69037 -0.19130

33
SCF Energy = -1908.44458648
Enthalpy 0K = -1908.217566
Enthalpy 298K = -1908.196550
Free Energy 298K = -1908.270744
Lowest Frequencies = 8.0949 cm-1
ASQ8c_a
C 5.50061 -1.40281 -0.00000
C 4.40032 -2.25427 -0.00000
C 3.12088 -1.71457 -0.00000
C 2.92248 -0.32181 -0.0000

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