SUPPLEMENTARY INFORMATION

Pyrazolyl-functionalised Ag(I)-NHC complexes: synthesis, characterisation, antibacterial, and computational investigation

Ngonidzashe Ruwizhi,[a] Karen Pillay,[b] Janade Moodley,[b] Thishana Singh,[a] Bernard Omondi,[a] and Muhammad D. Bala*[a]

[a] School of Agriculture and Science, Discipline of Chemistry, University of KwaZulu-Natal, Westville Campus, Private Bag X54001, Durban 4000, South Africa

[b] School of Agriculture and Science, Discipline of Biological Sciences, University of KwaZulu-Natal, Westville Campus, Private Bag X54001, Durban 4000, South Africa

*E-mail: bala@ukzn.ac.za

Contents

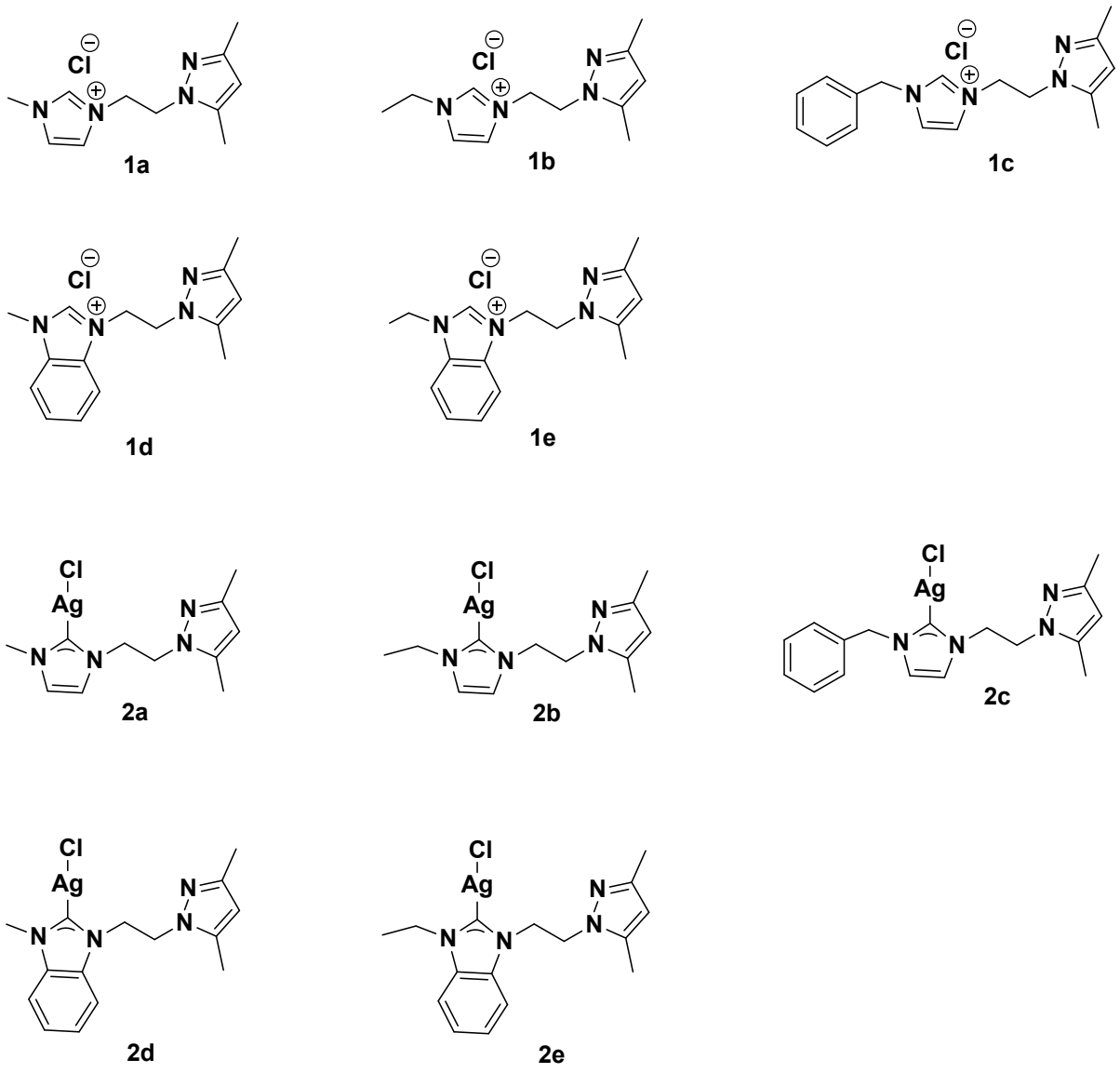

Figure S1: Structures of compounds **1a-e** and **2a-e.**

NMR Spectra

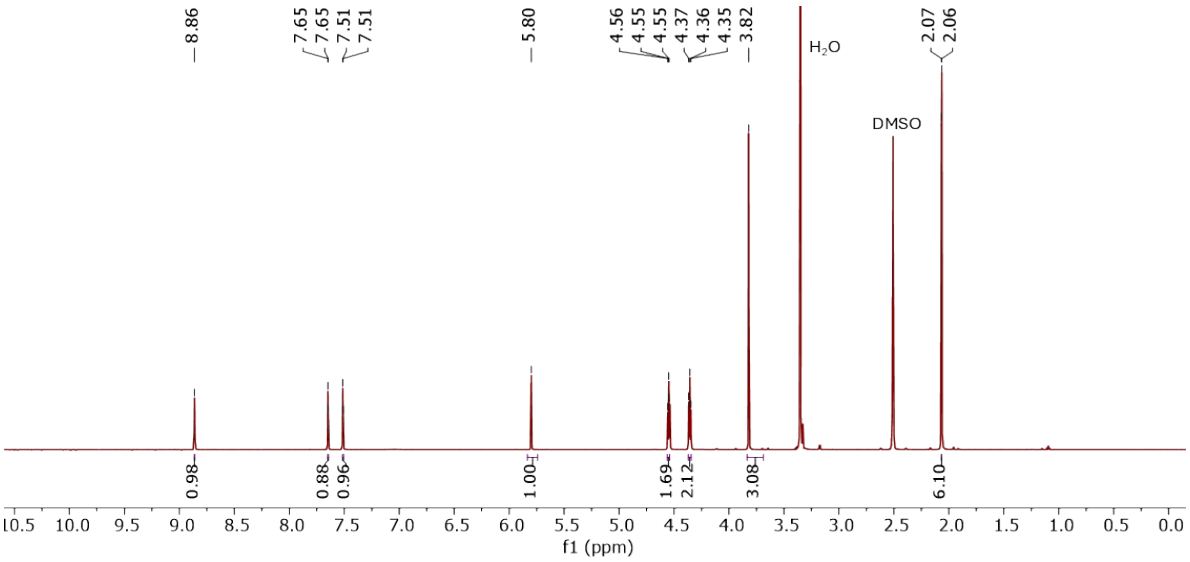

Figure S2:[1]H-NMR spectrum for **1a**.

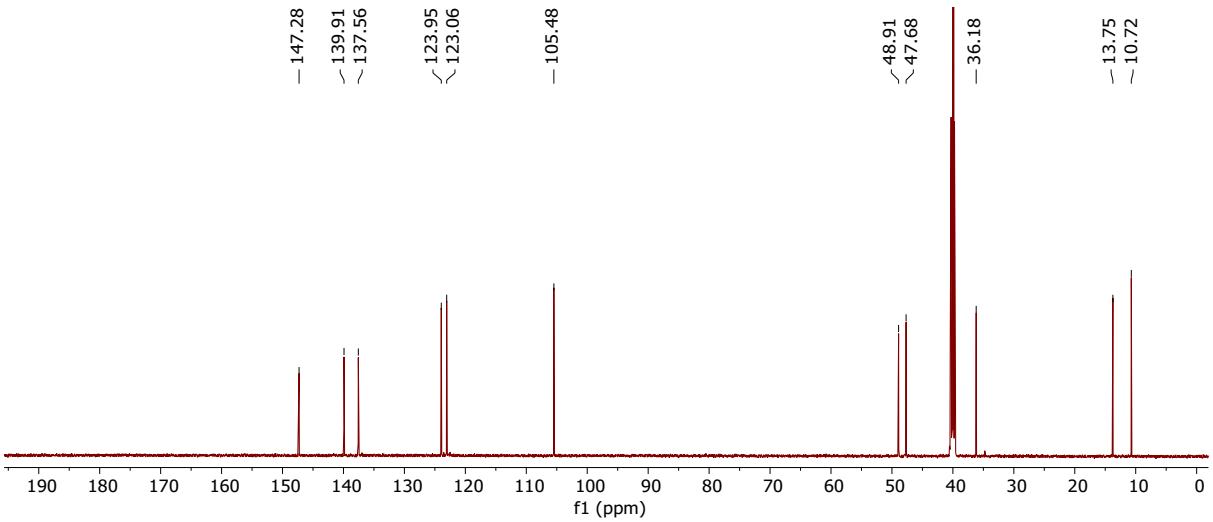

Figure S3: [13]C-NMR spectrum for **1a**.

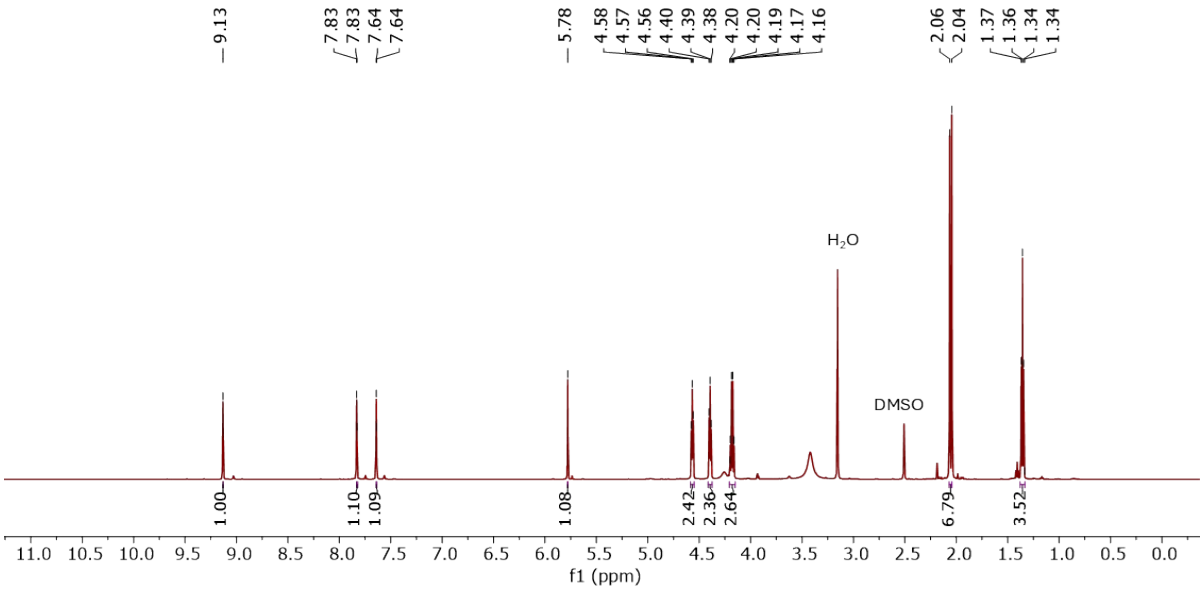

Figure S4: [1]H-NMR spectrum for **1b**.

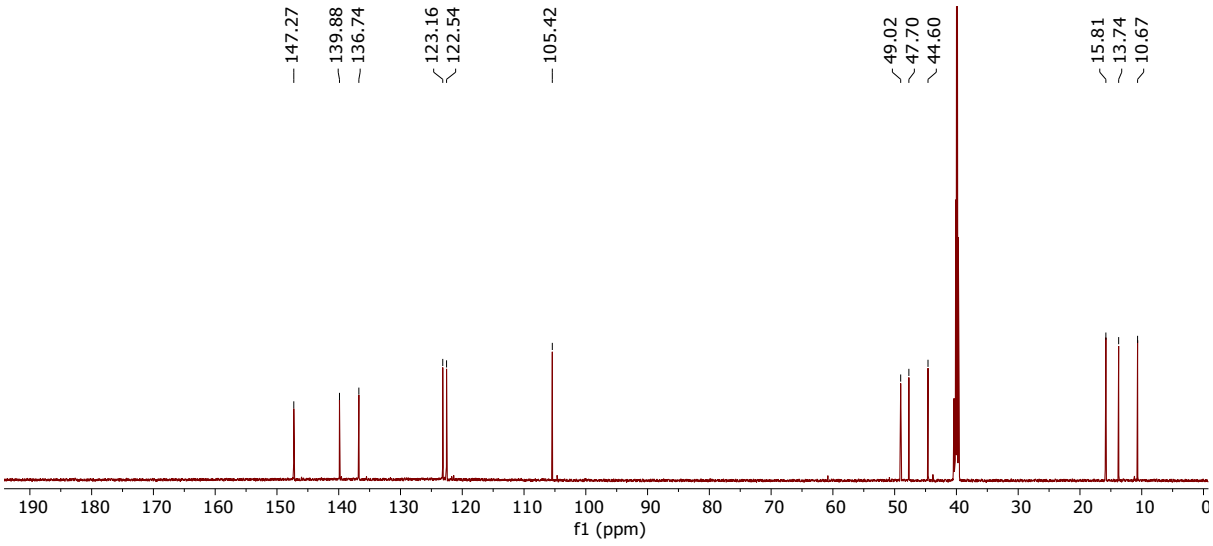

Figure S5: [13]C-NMR spectrum for **1b**.

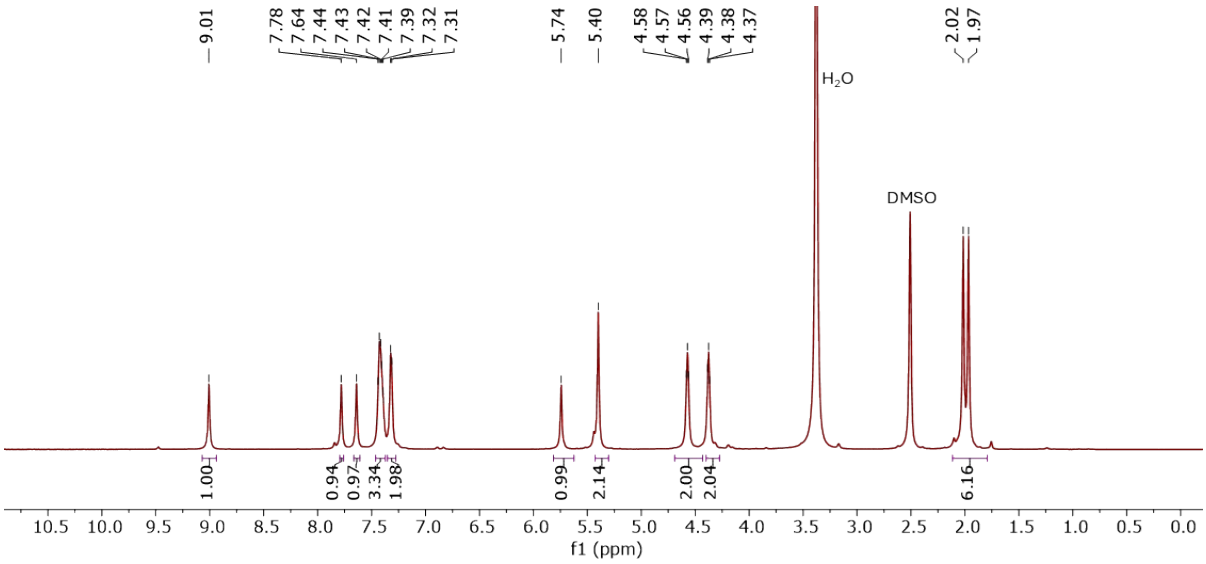

Figure S6: ^{1}H-NMR spectrum for **1c**.

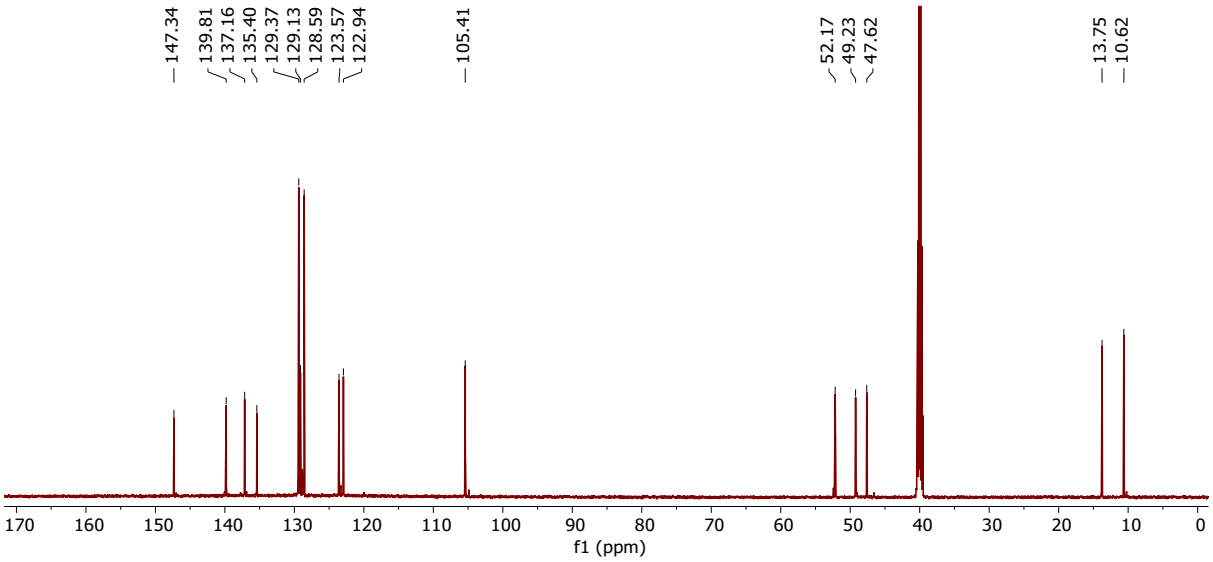

Figure S7: ^{13}C-NMR spectrum for **1c**.

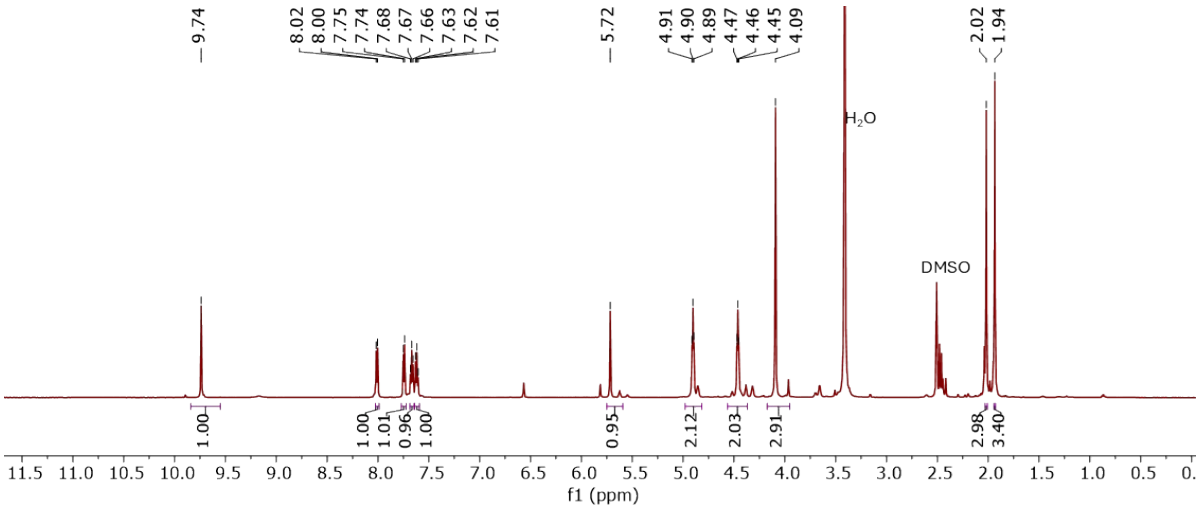

Figure S8: ^{1}H-NMR spectrum for **1d**.

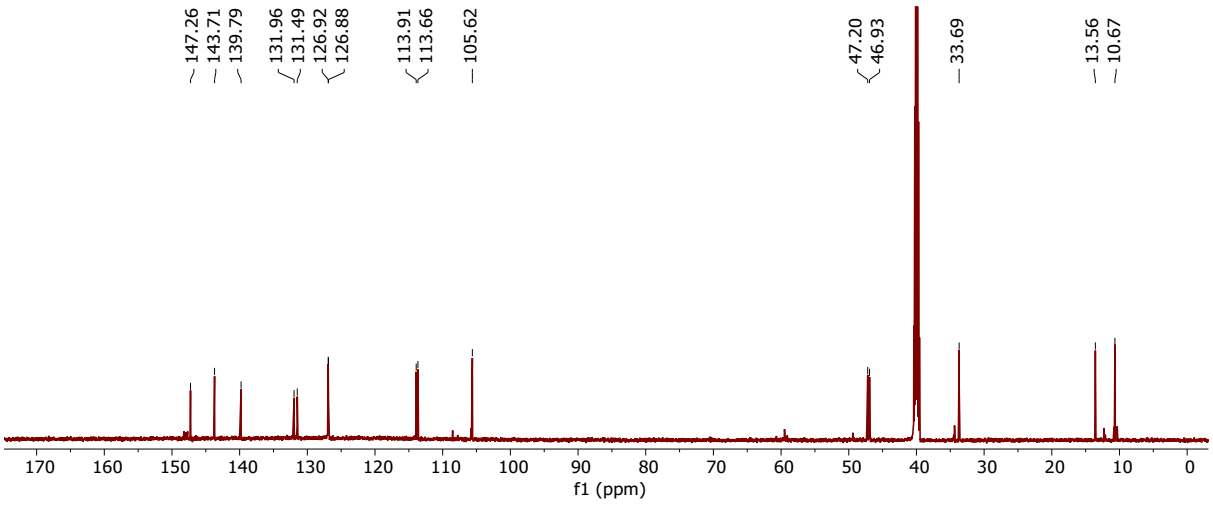

Figure S9: ^{13}C-NMR spectrum for **1d**.

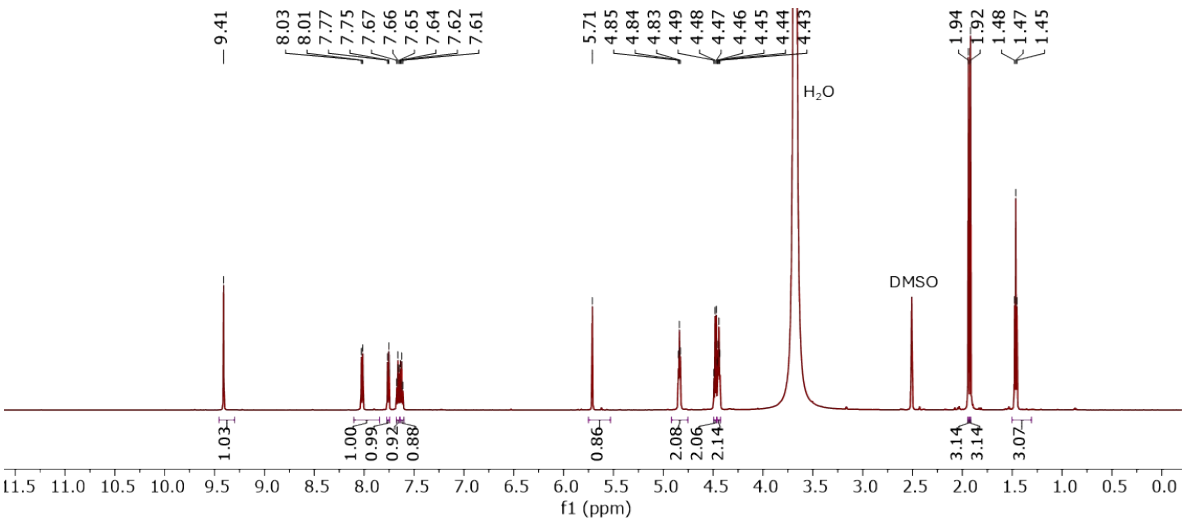

Figure S10: ^{1}H-NMR spectrum for **1e**.

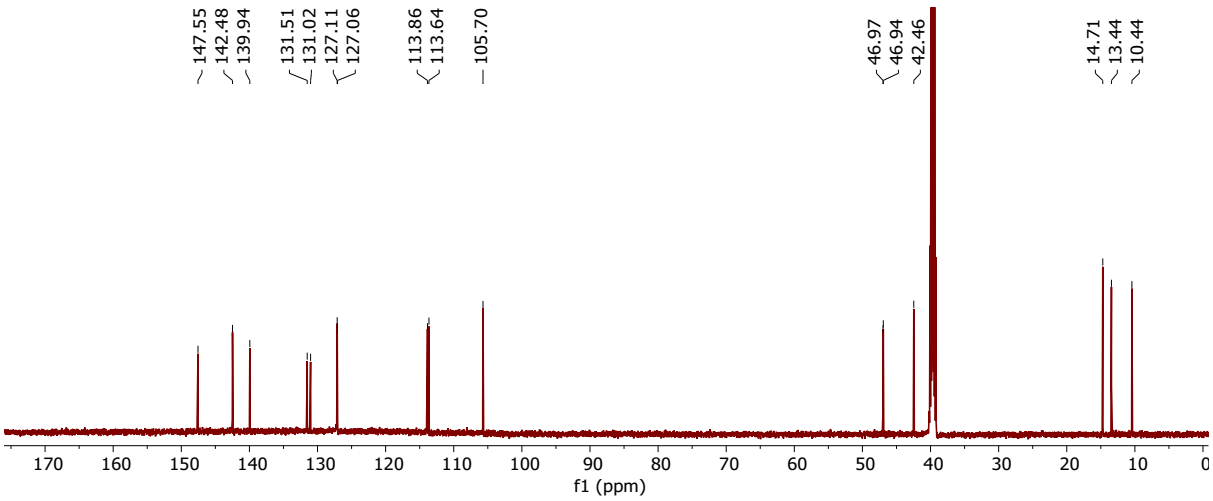

Figure S11: ^{13}C-NMR spectrum for **1e**.

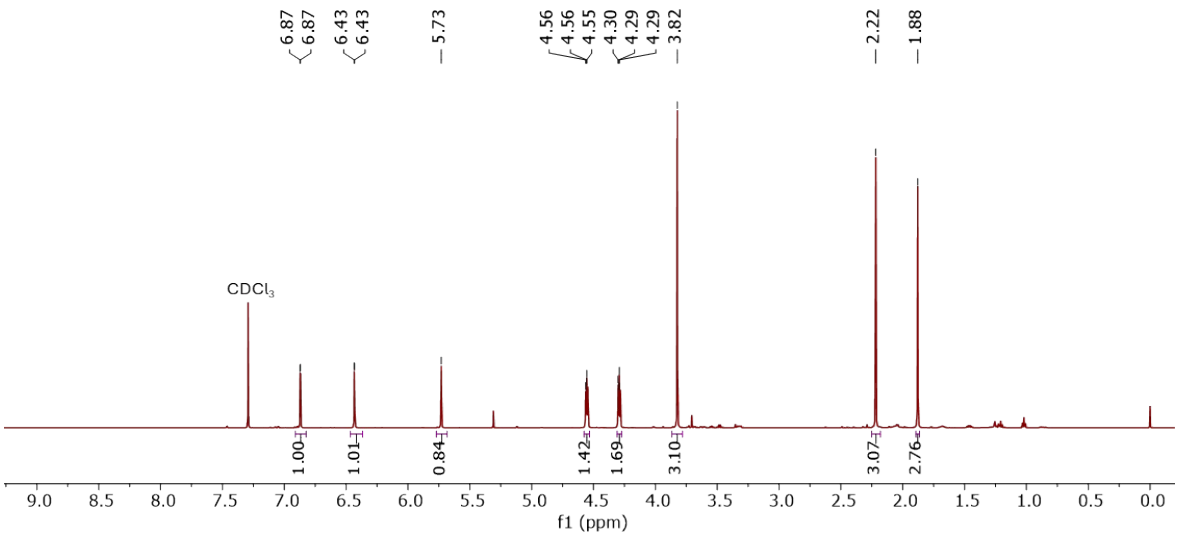

Figure S12: ^{1}H-NMR spectrum for **2a**.

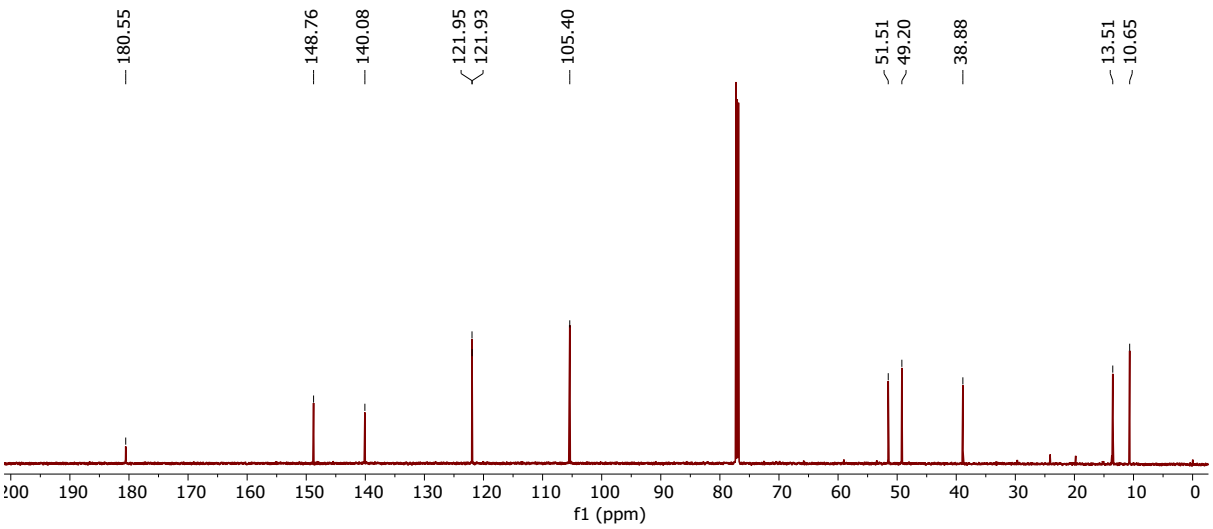

Figure S13: ^{13}C-NMR spectrum for **2a**.

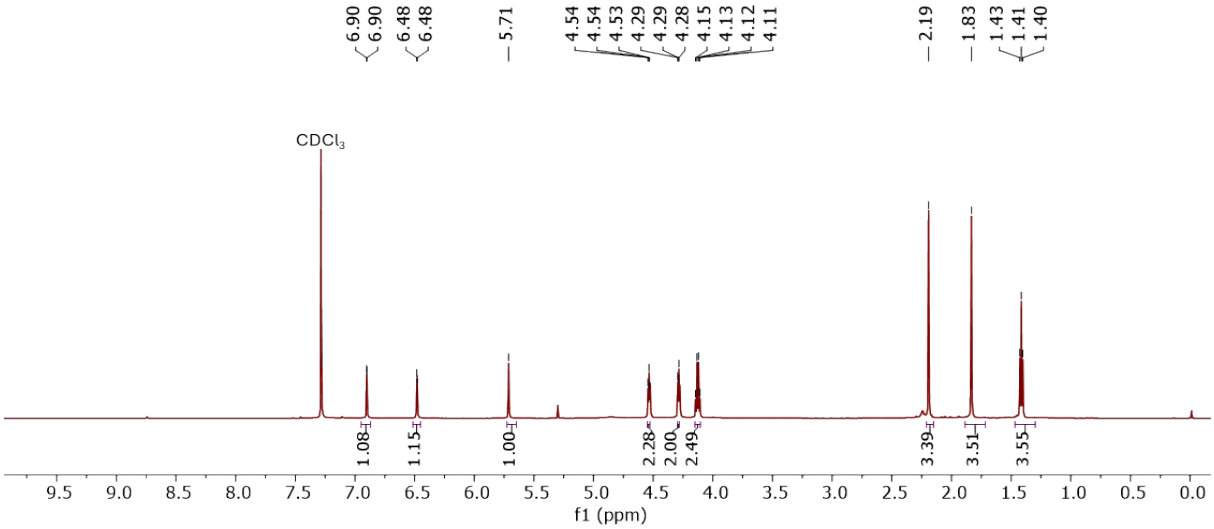

Figure S14: ^{1}H-NMR spectrum for **2b**.

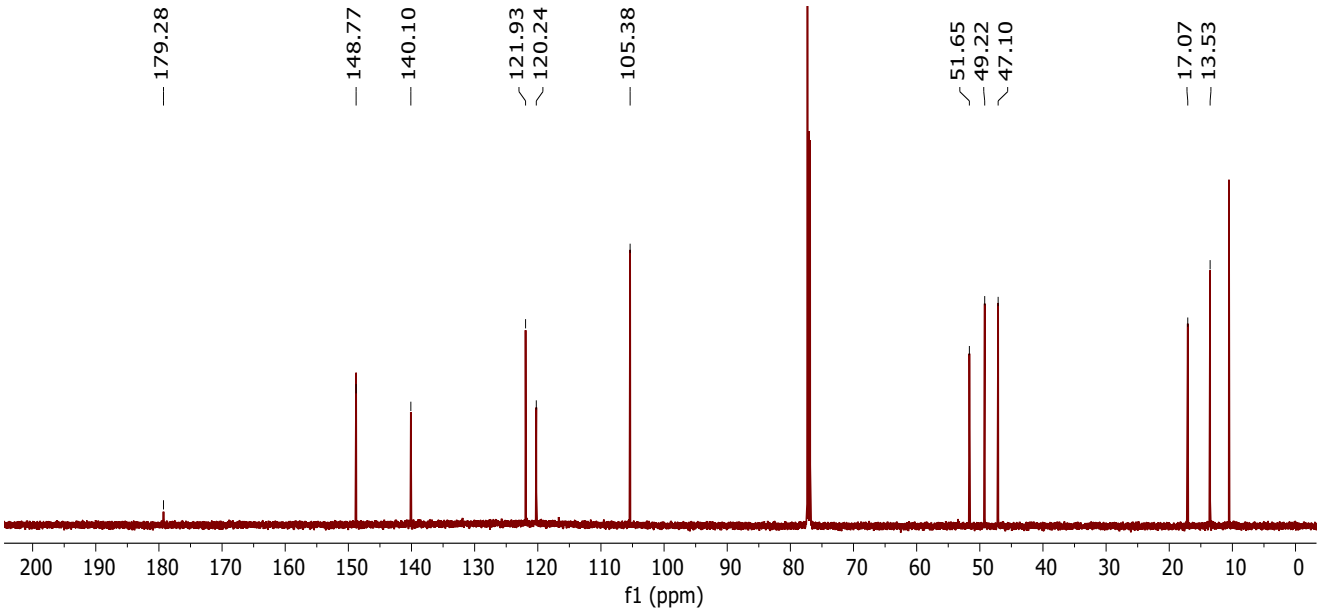

Figure S15: ^{13}C-NMR spectrum for **2b**.

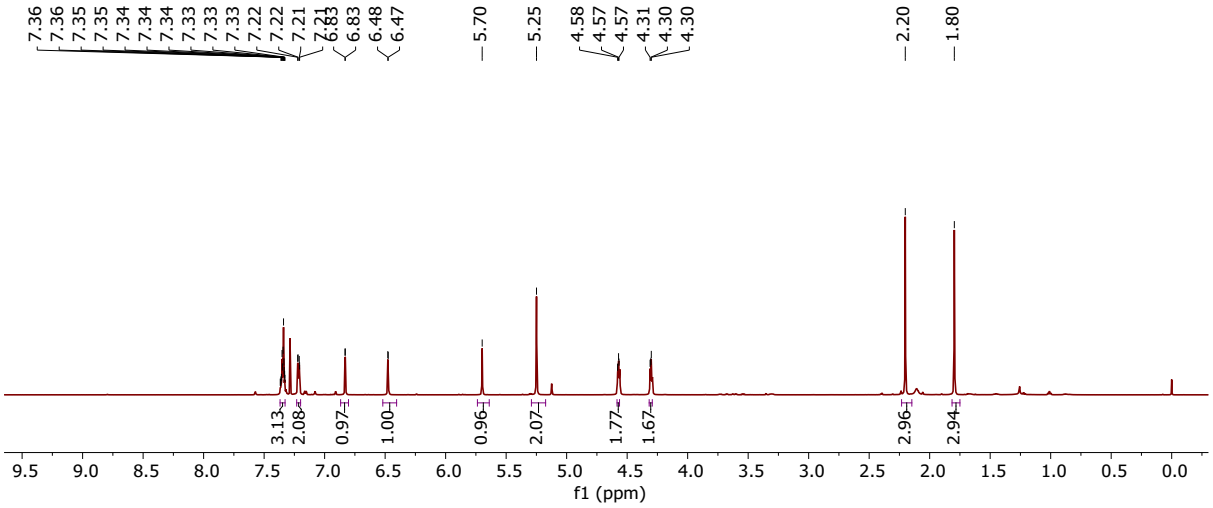

Figure S16: ^{1}H-NMR spectrum for **2c**.

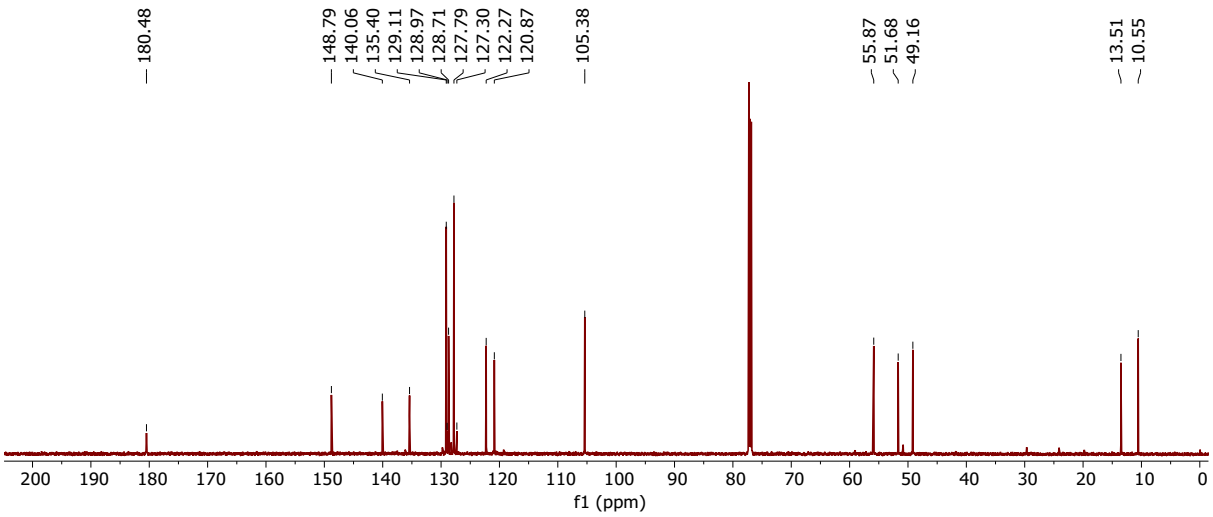

Figure S17: ^{13}C-NMR spectrum for **2c**.

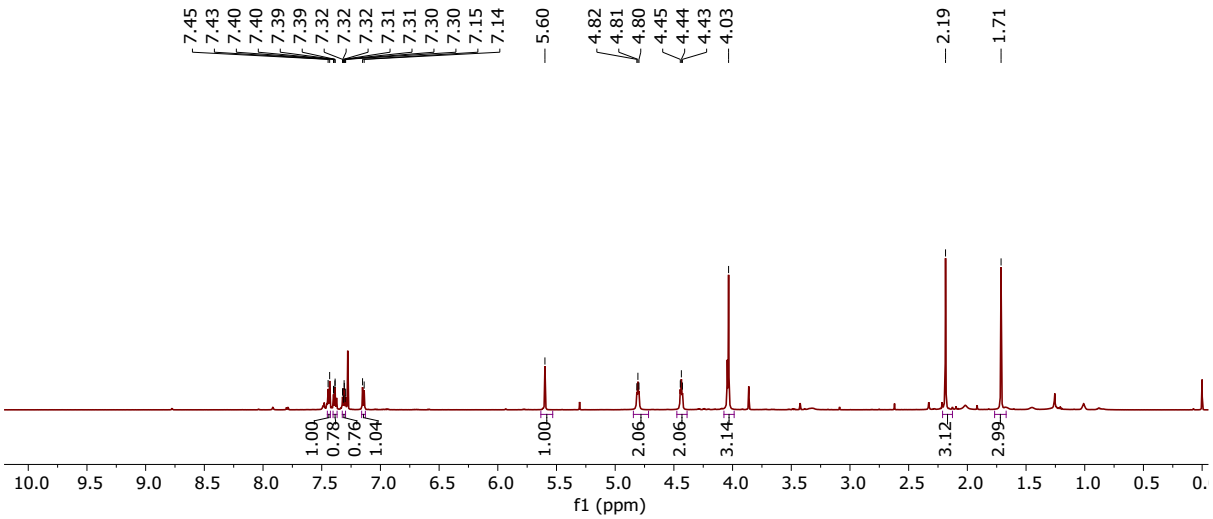

Figure S18: ^{1}H-NMR spectrum for **2d**.

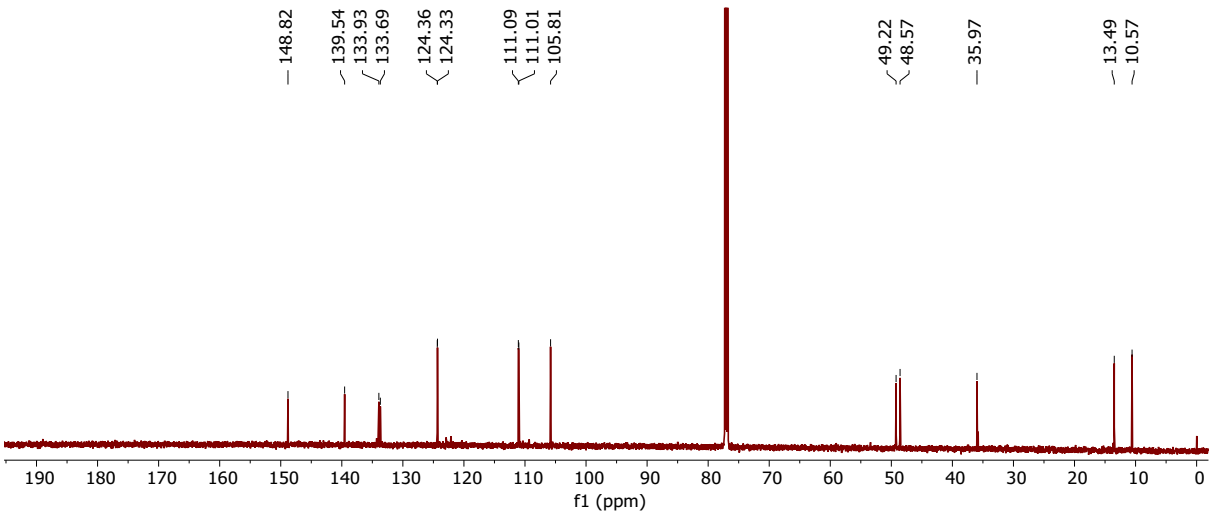

Figure S19: ^{13}C-NMR spectrum for **2d**.

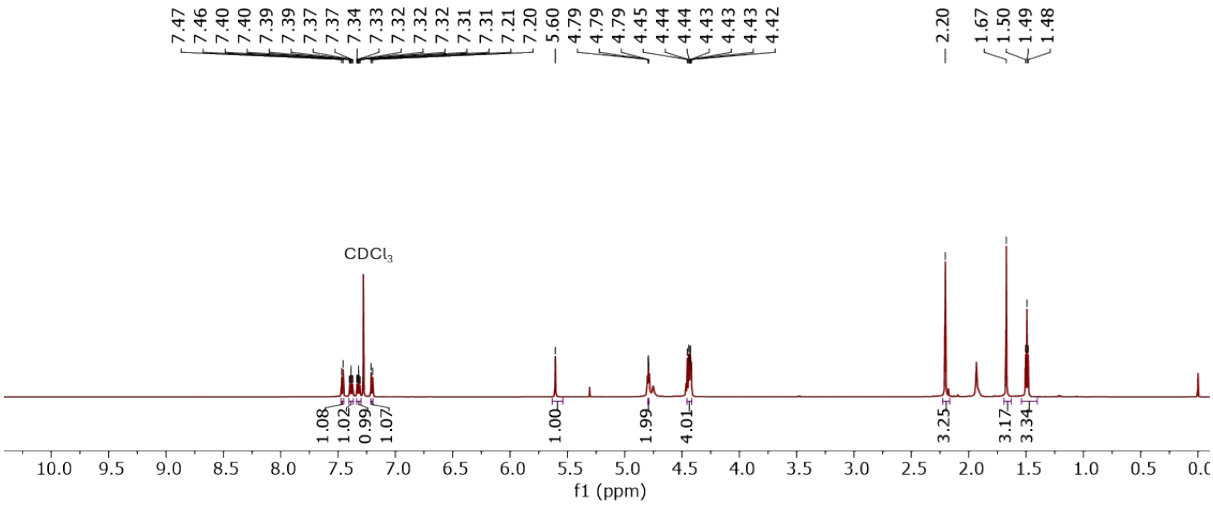

Figure S20: [1]H-NMR spectrum for **2e**.

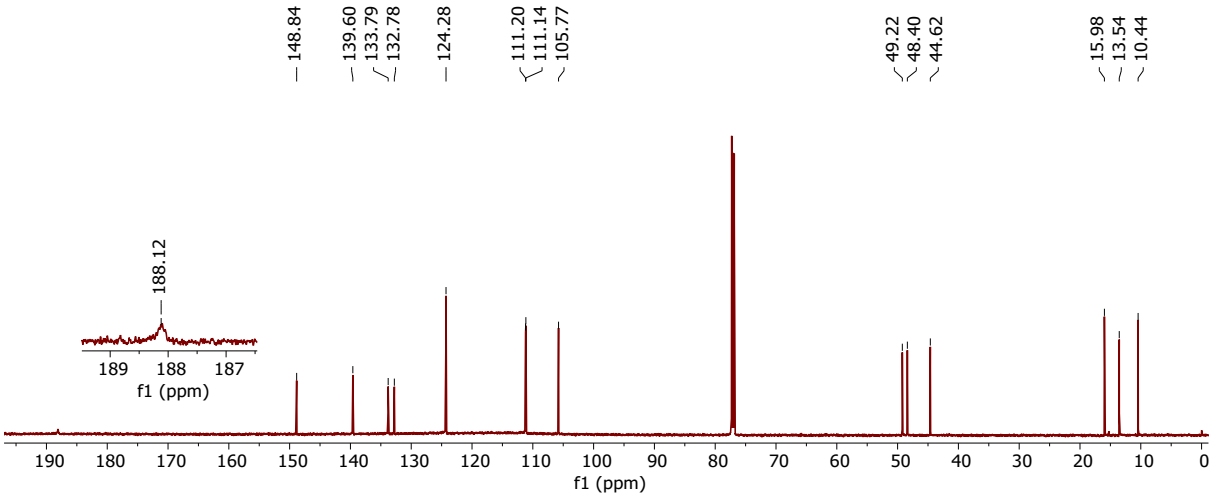

Figure S21: [13]C-NMR spectrum for **2e**.

LRMS spectra of compounds

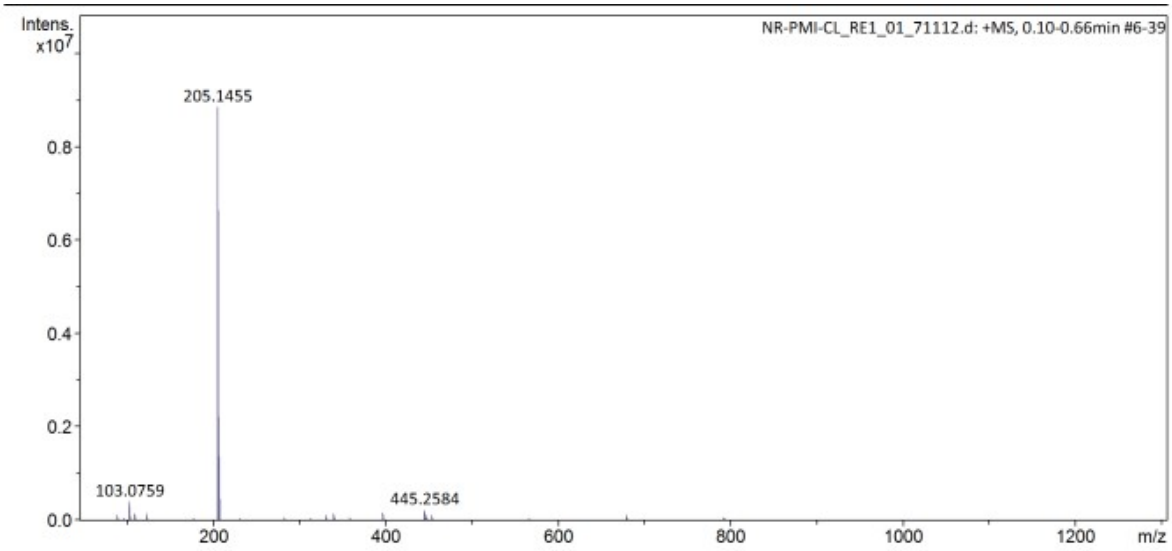

Figure S22: LRMS spectrum for **1a**.

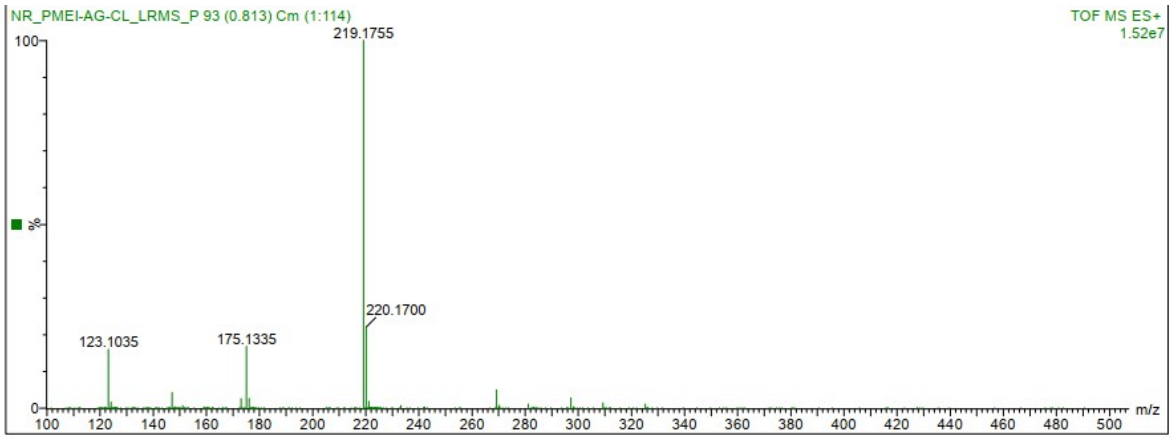

Figure S23: LRMS spectrum for **1b**.

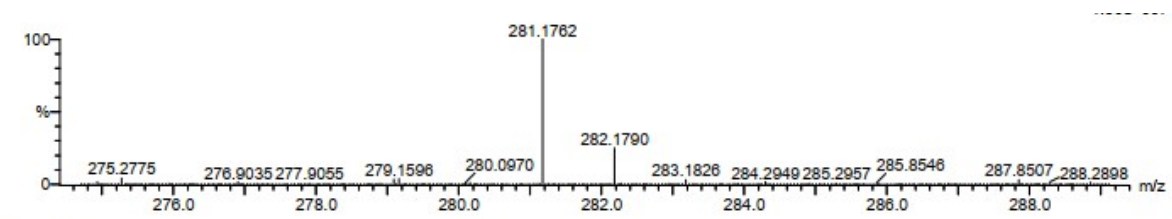

Figure S24: LRMS spectrum for **1c**.

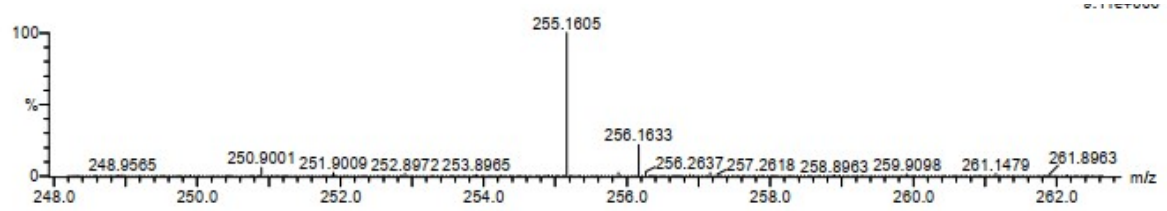

Figure S25: LRMS spectrum for **1d**.

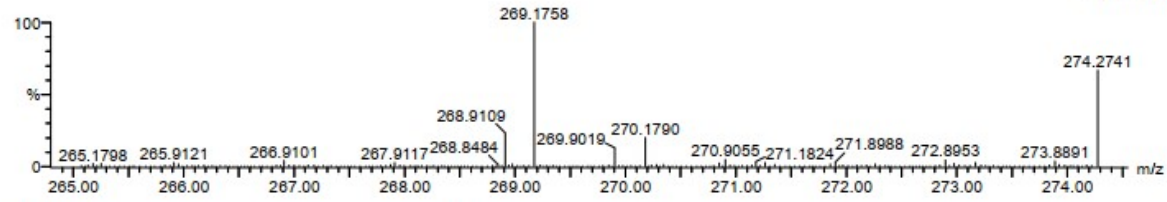

Figure S26: LRMS spectrum for **1e**.

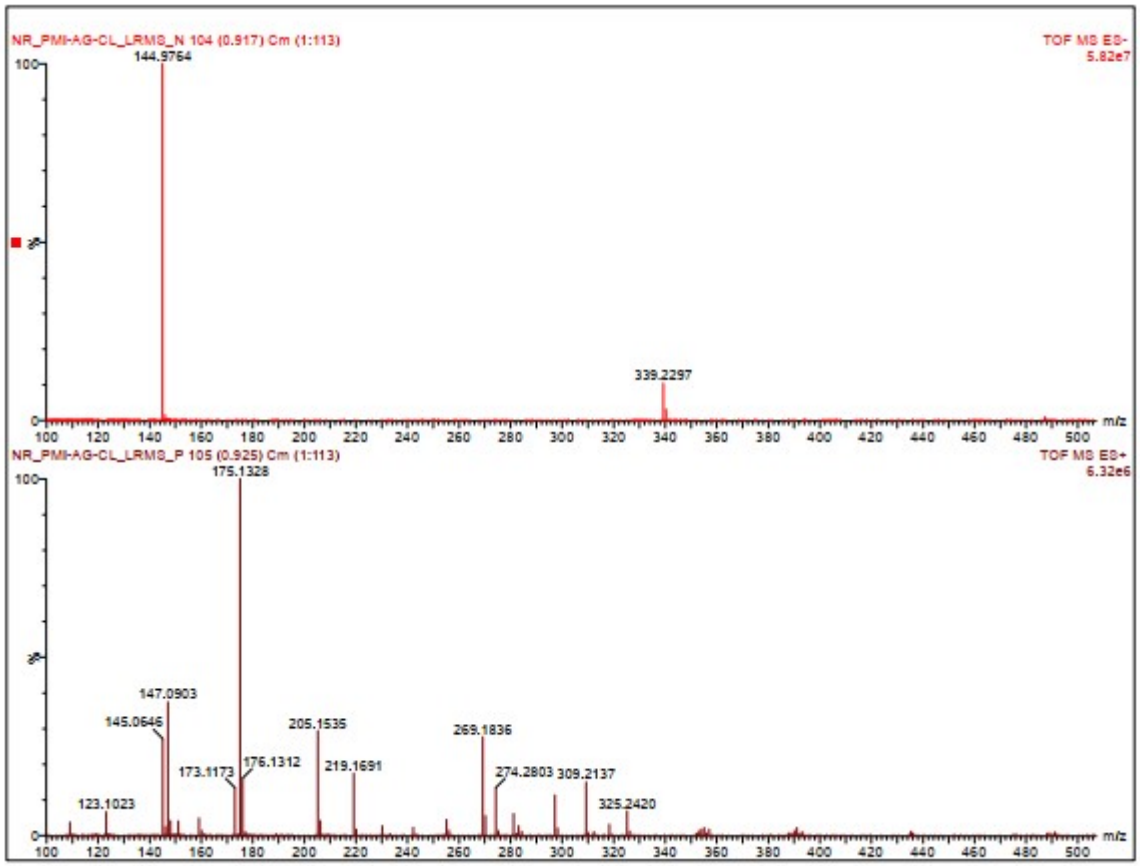

Figure S27: LRMS spectrum for **2a**.

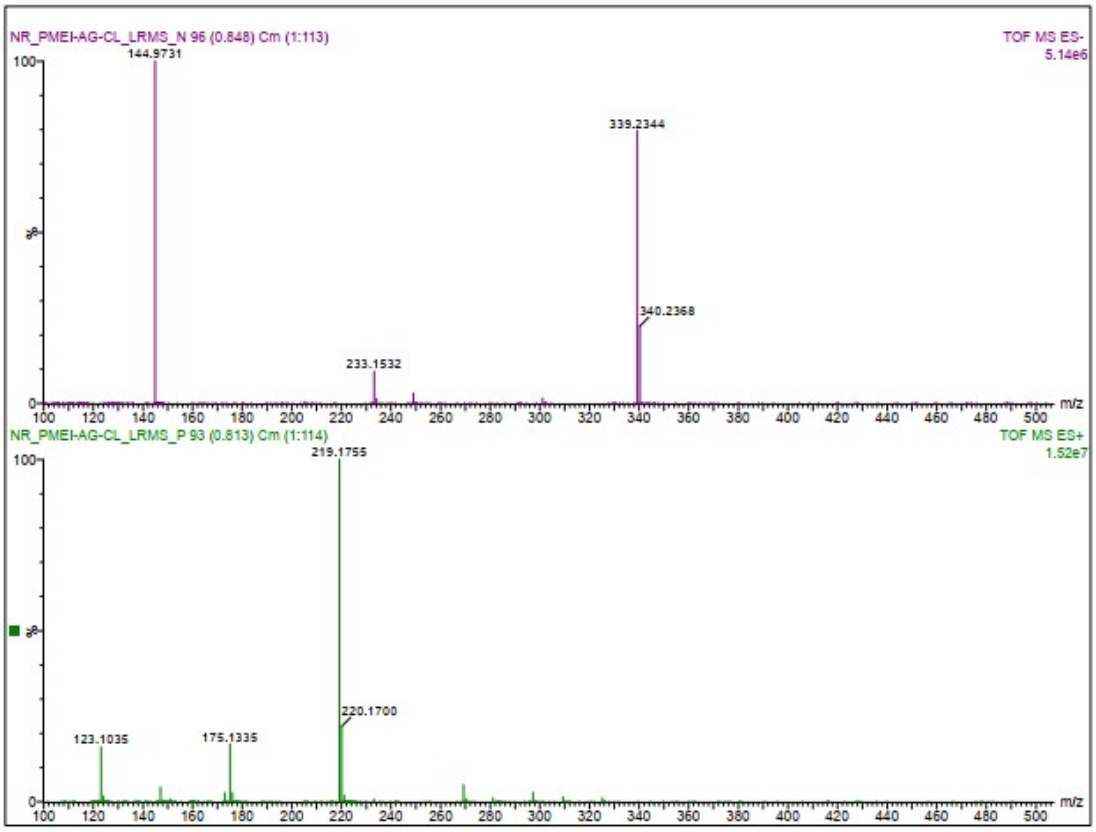

Figure S28: LRMS spectrum for **2b**.

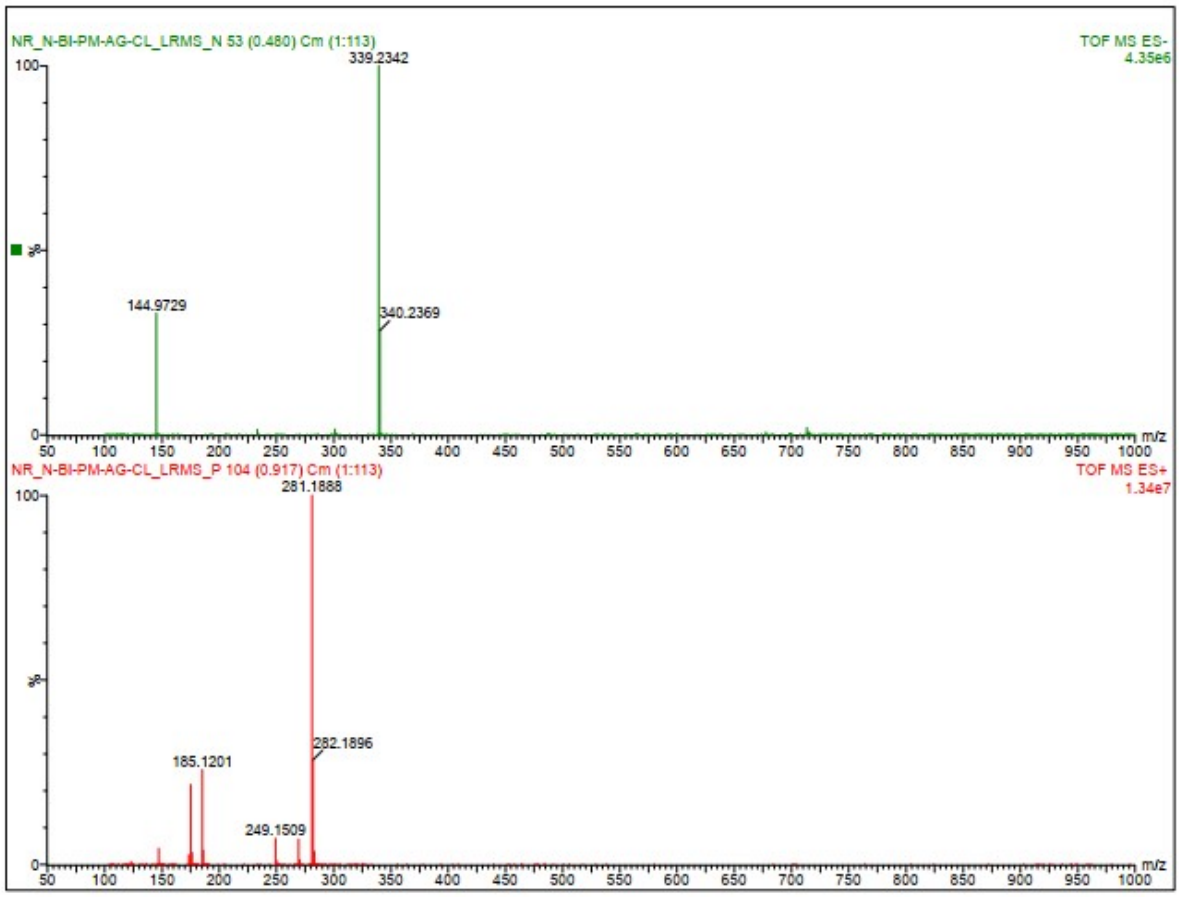

Figure S29: LRMS spectrum for **2c**.

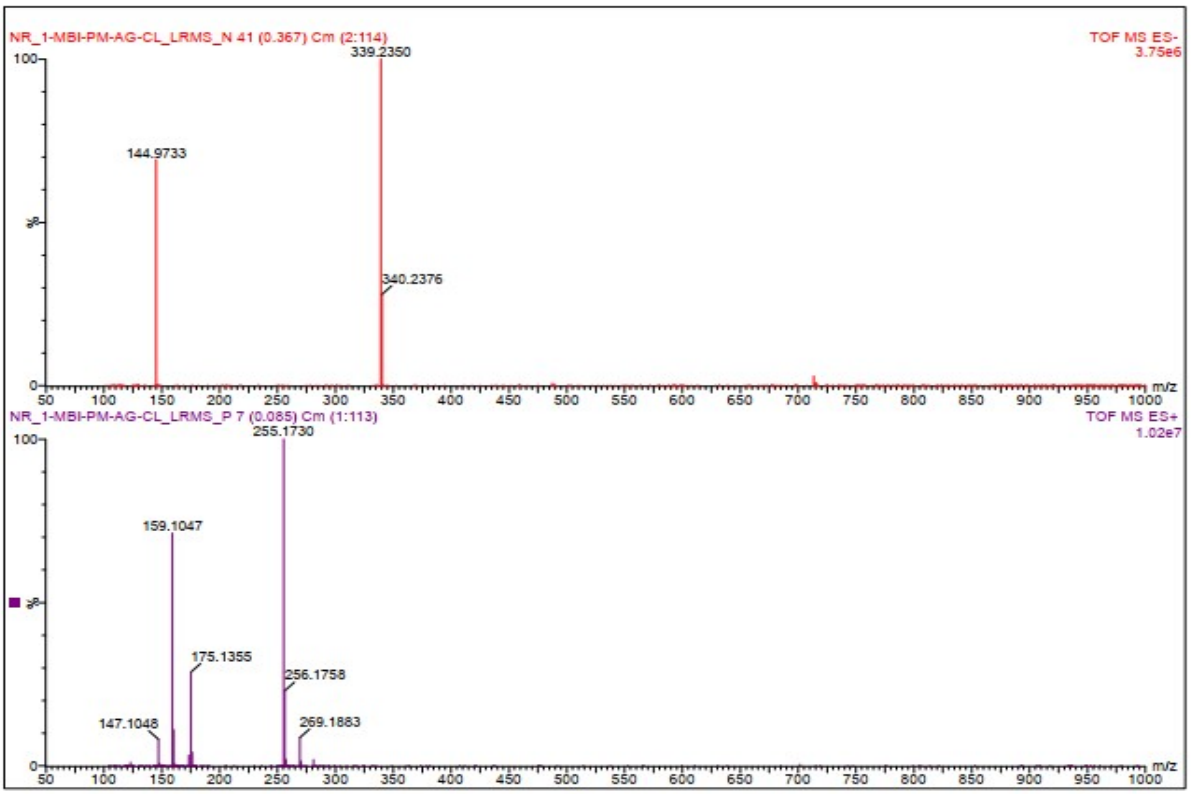

Figure S30: LRMS spectrum for **2d**.

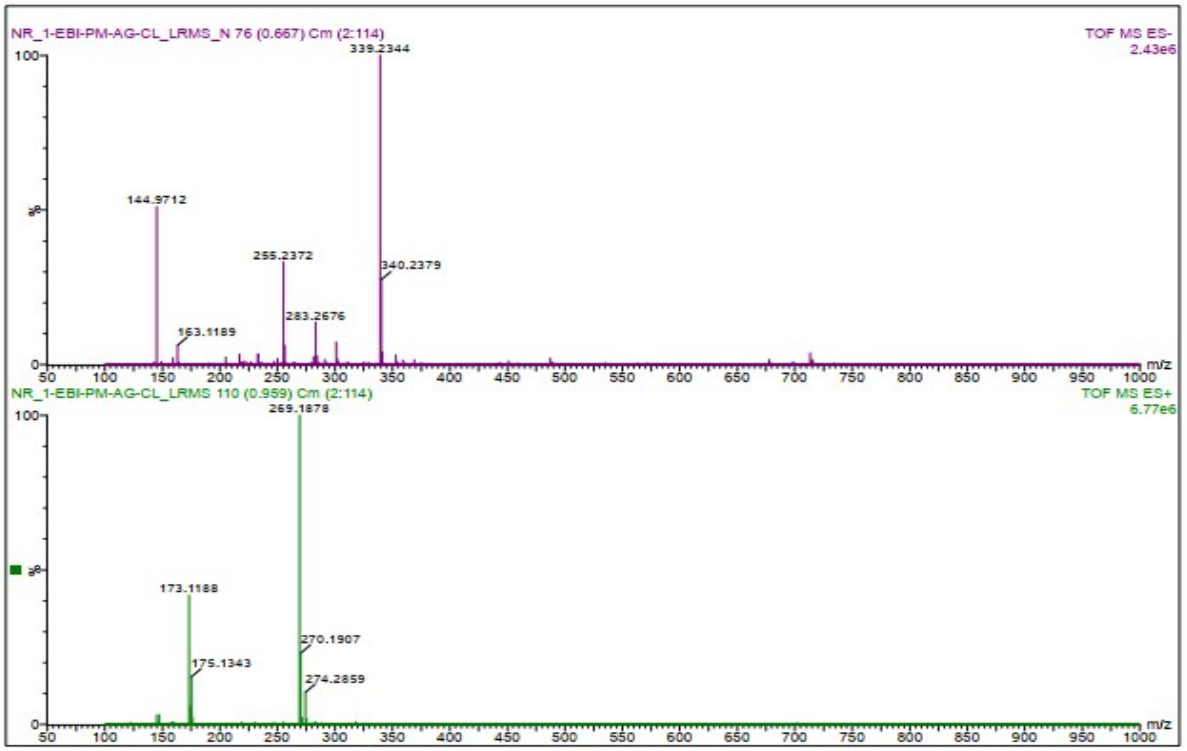

Figure S31: LRMS spectrum for **2e**.

Experimental and simulated IR Spectra of compounds

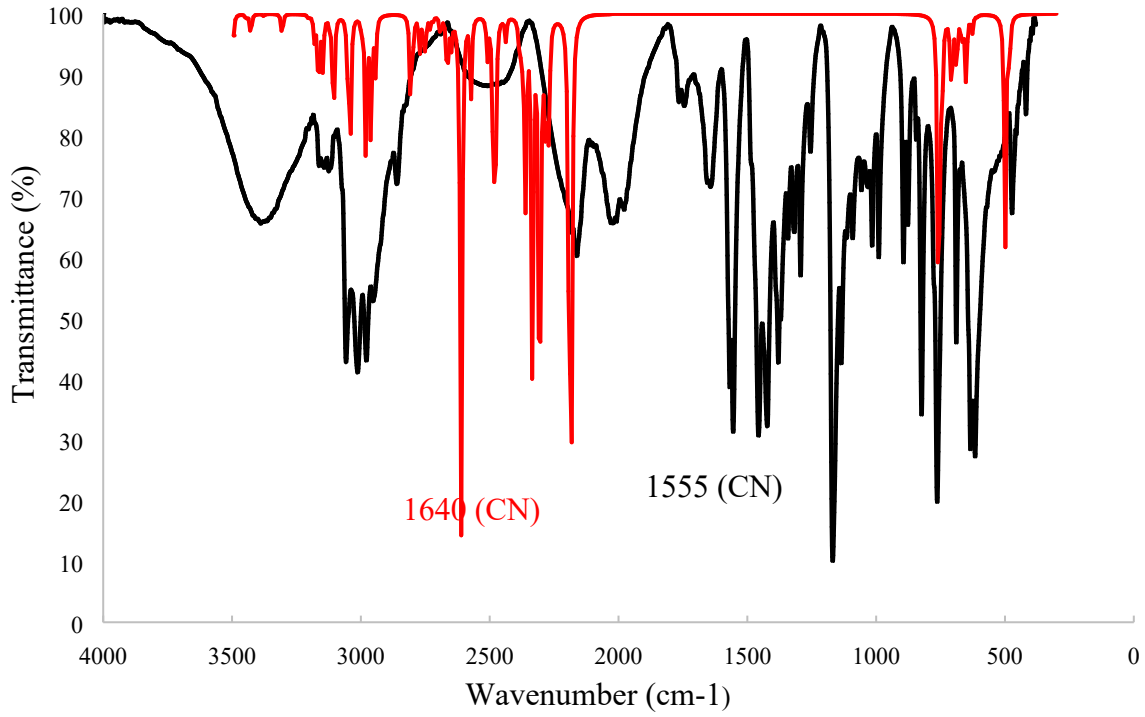

Figure S32: Simulated (red) and experimental (black) IR spectra of **1a**.

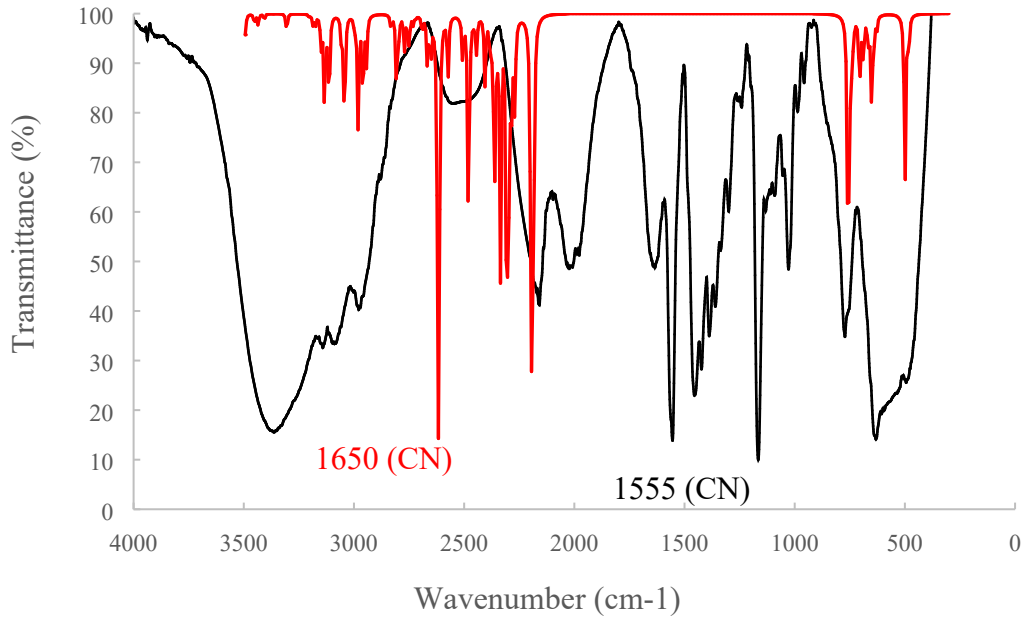

Figure S33: Simulated (red) and experimental (black) IR spectra of **1b**.

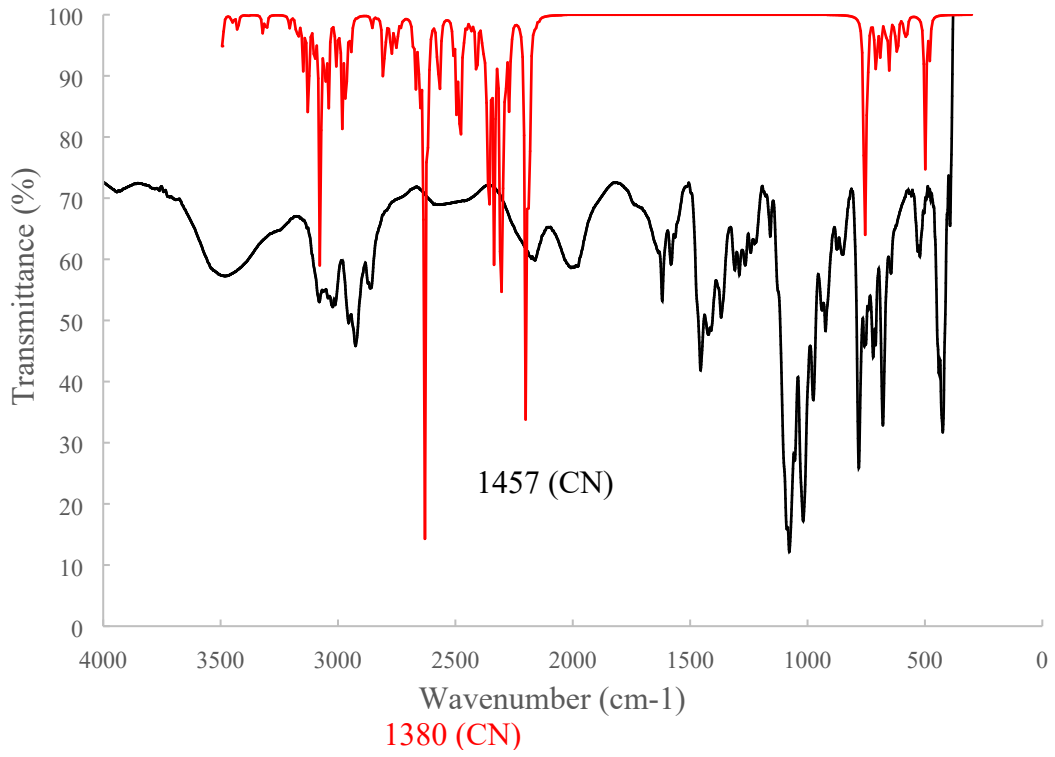

Figure S34: Simulated (red) and experimental (black) IR spectra of **1c**.

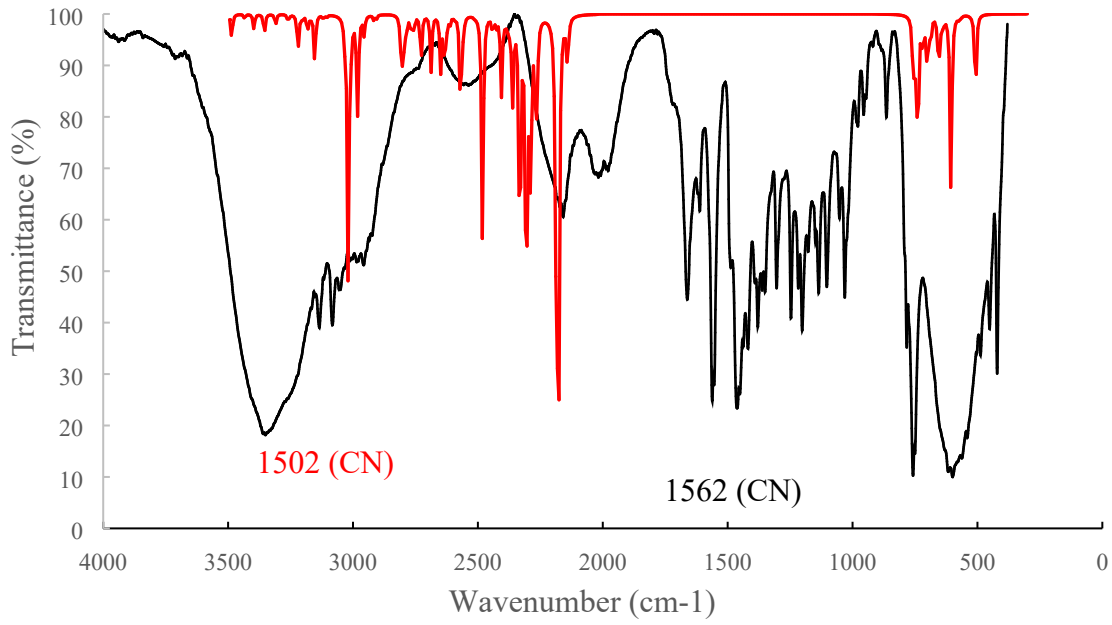

Figure S35: Simulated (red) and experimental (black) IR spectra of **1d**.

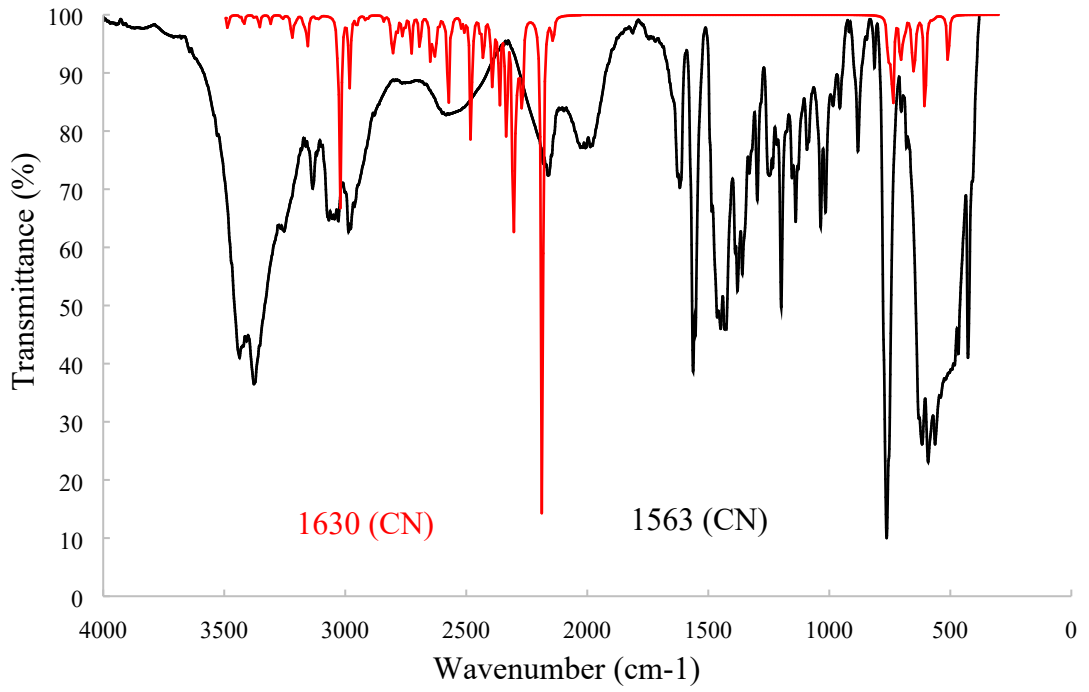

Figure S36: Simulated (red) and experimental (black) IR spectra of **1e**.

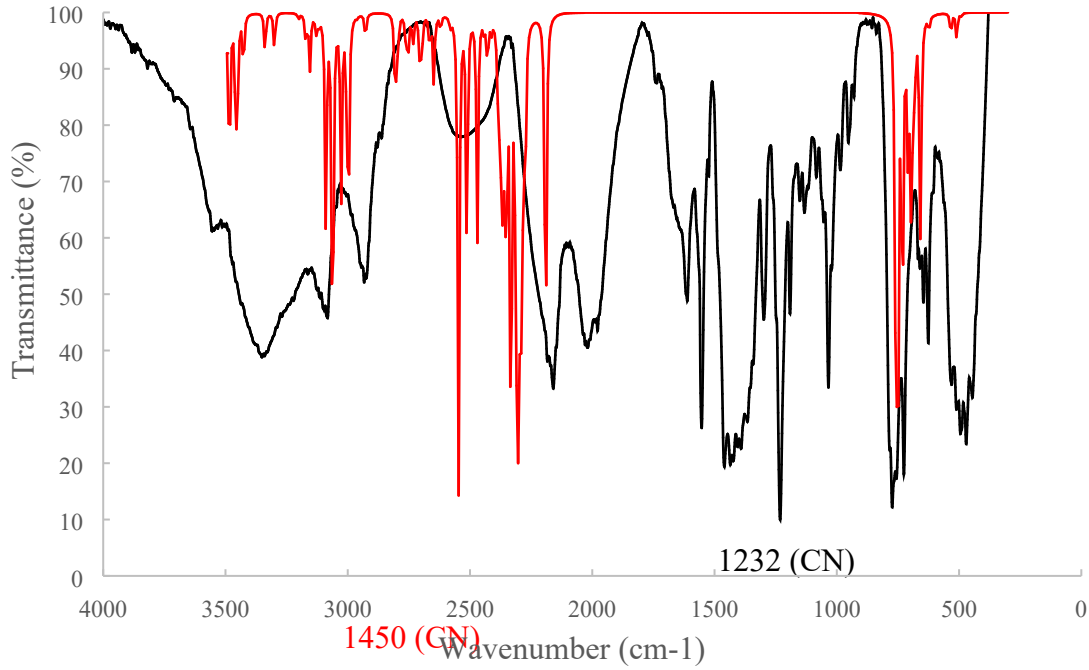

Figure S37: Simulated (red) and experimental (black) IR spectra of **2a**.

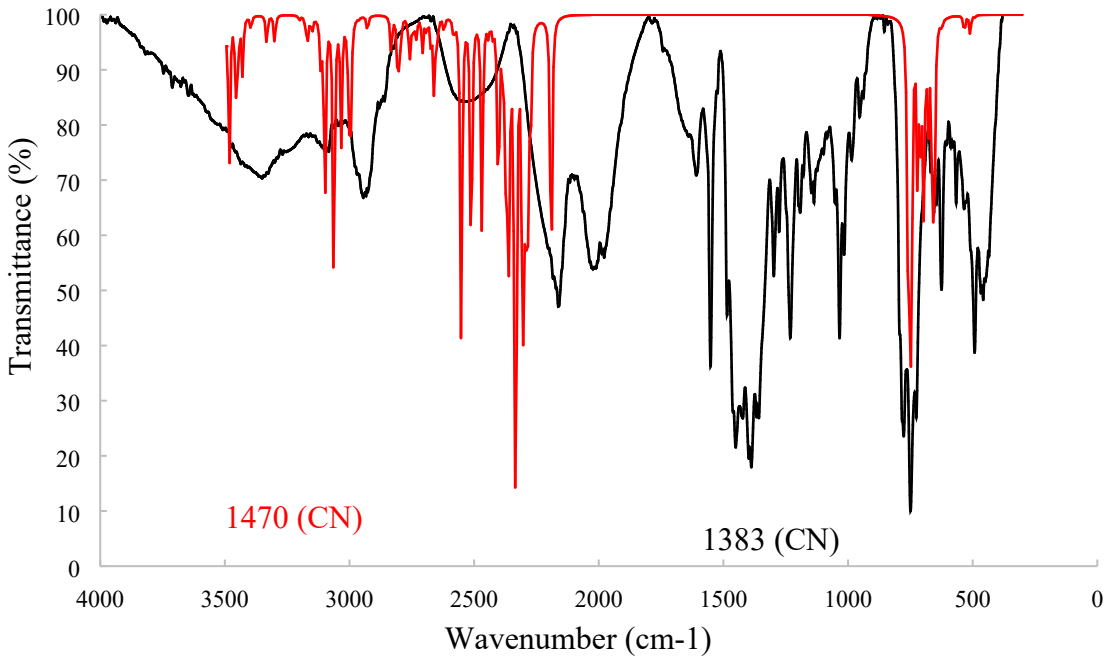

Figure S38: Simulated (red) and experimental (black) IR spectra of **2b**.

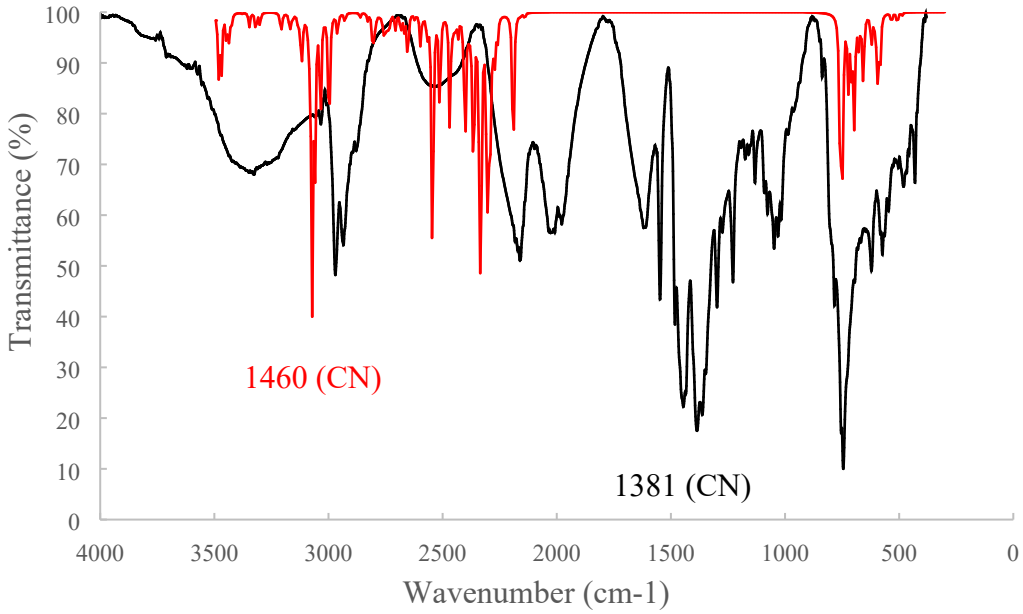

Figure S39: Simulated (red) and experimental (black) IR spectra of **2c**.

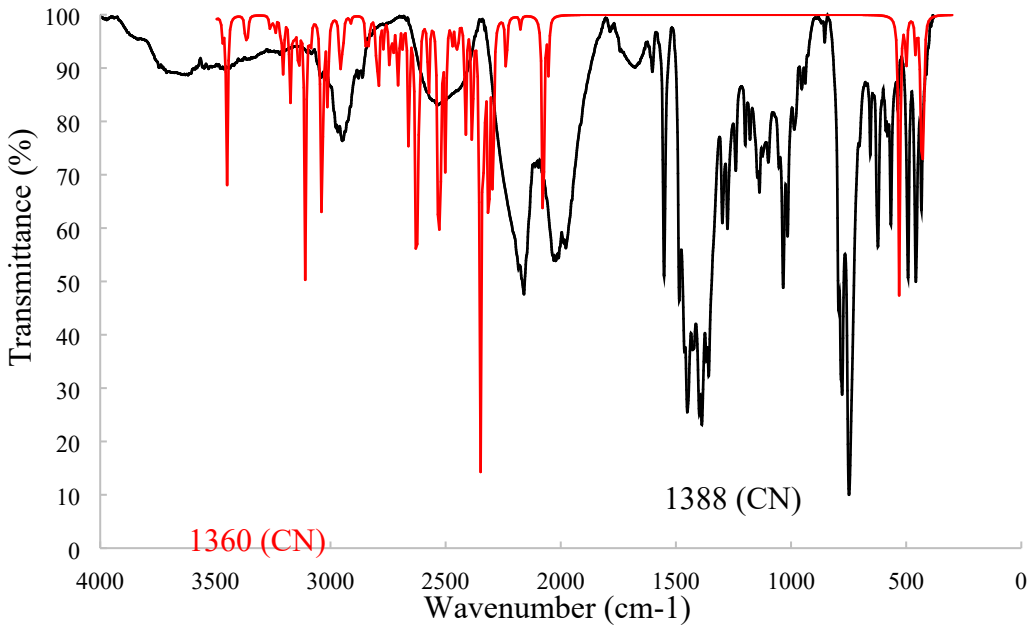

Figure S40: Simulated (red) and experimental (black) IR spectra of **2d**.

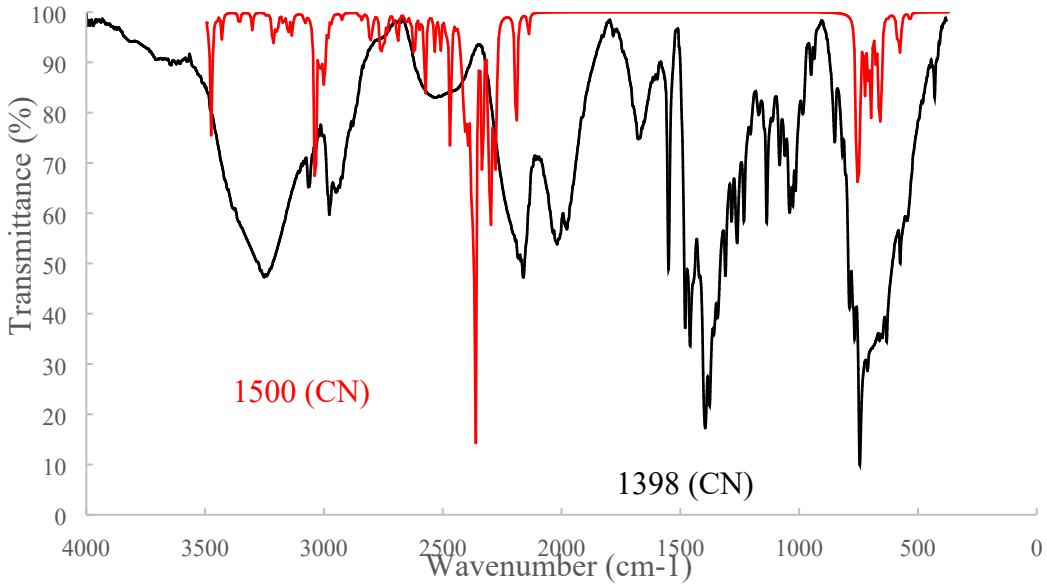

Figure S41: Simulated (red) and experimental (black) IR spectra of **2e**.

Experimental and simulated UV-Vis spectra of compounds

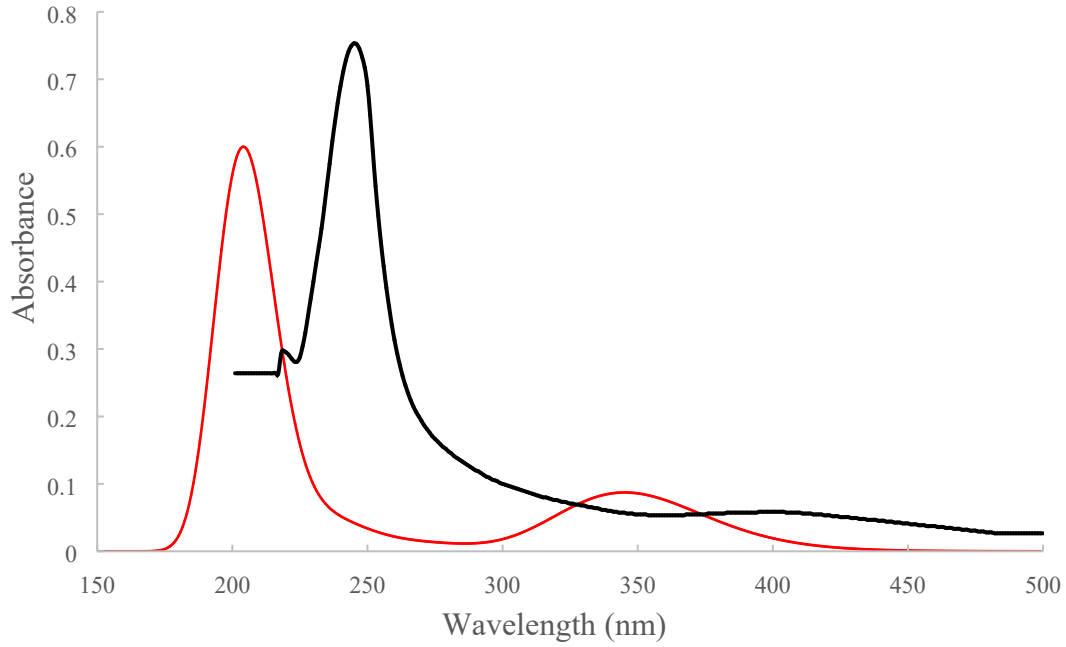

Figure S42: Simulated (red) and experimental (black)UV-vis spectra of **1a**.

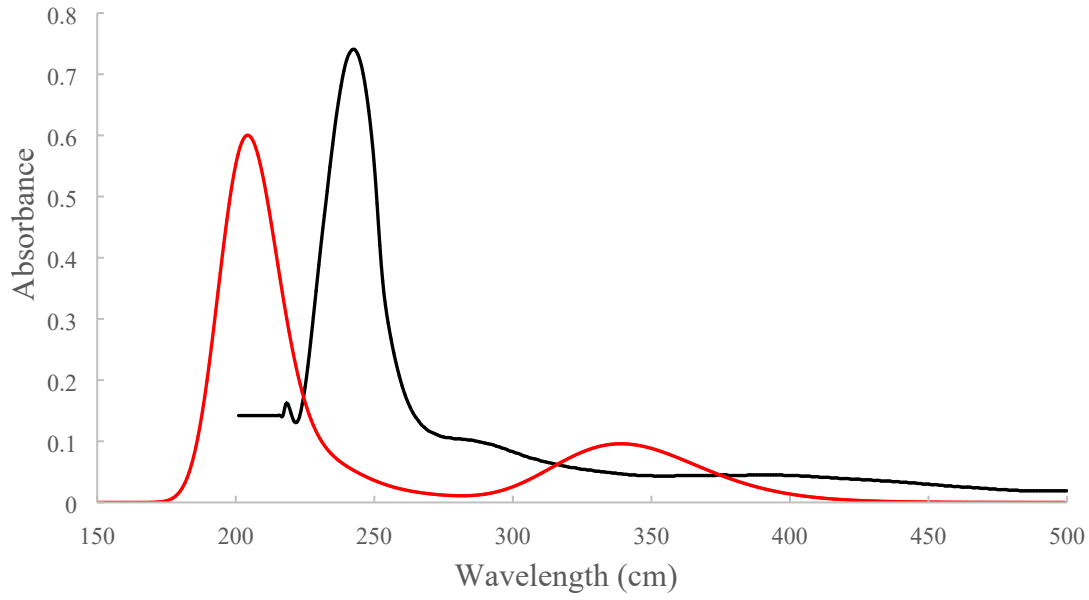

Figure S43: Simulated (red) and experimental (black)UV-vis spectra of **1b.**

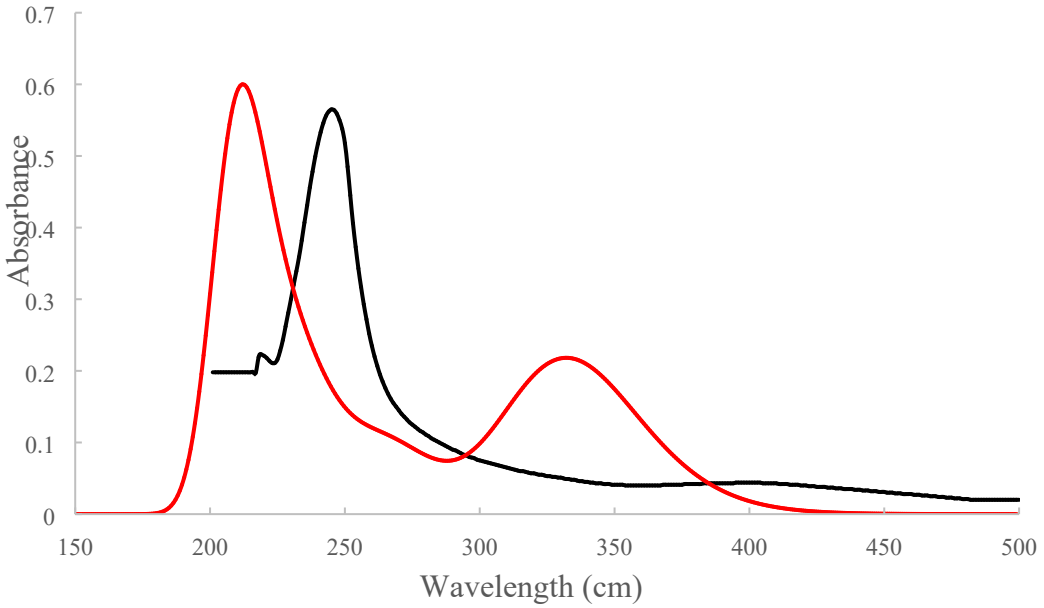

Figure S44: Simulated (red) and experimental (black)UV-vis spectra of **1c.**

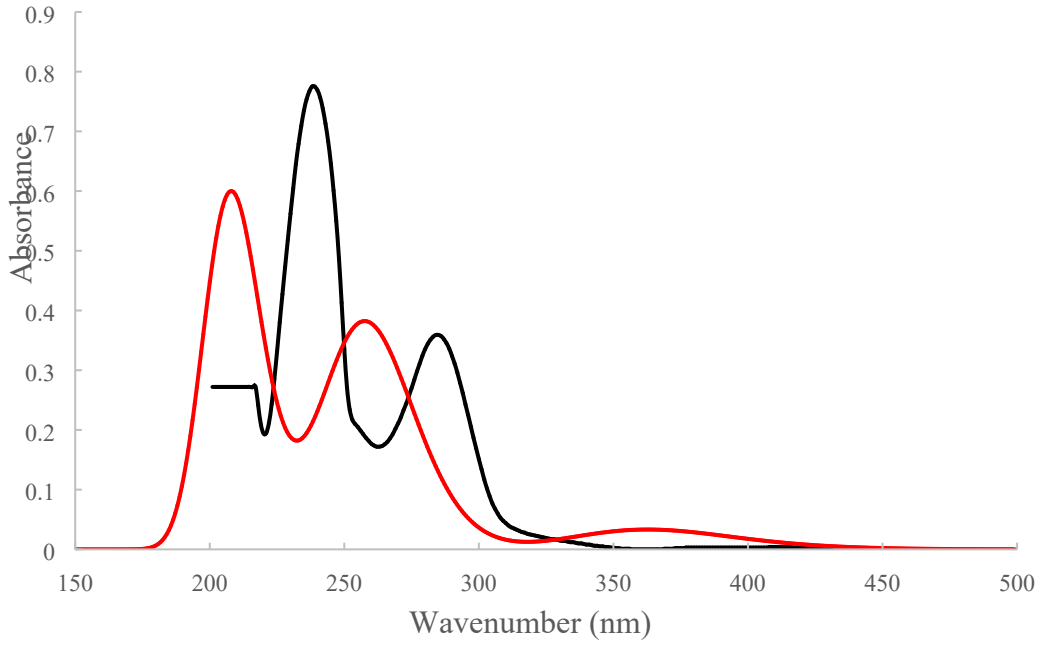

Figure S45: Simulated (red) and experimental (black)UV-vis spectra of **1d.**

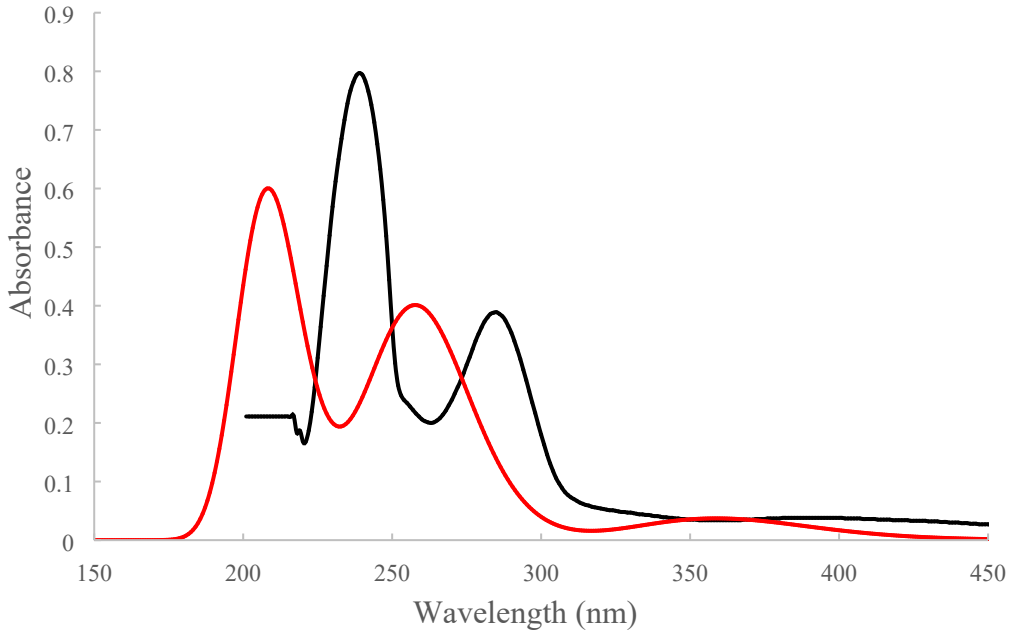

Figure S46: Simulated (red) and experimental (black)UV-vis spectra of **1e.**

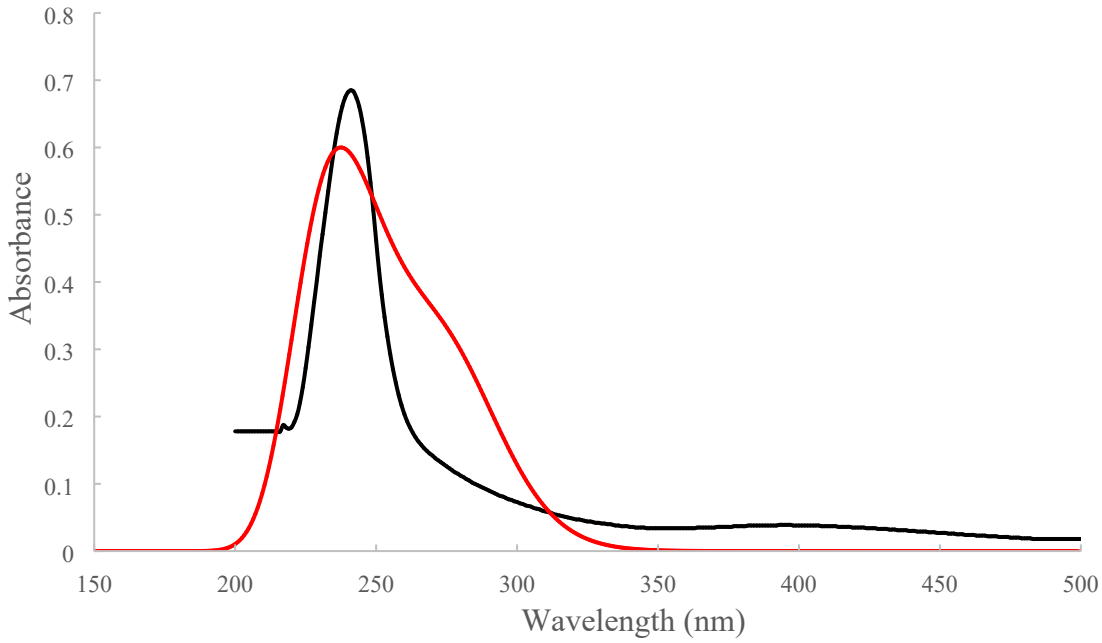

Figure S47: Simulated (red) and experimental (black)UV-vis spectra of **2a.**

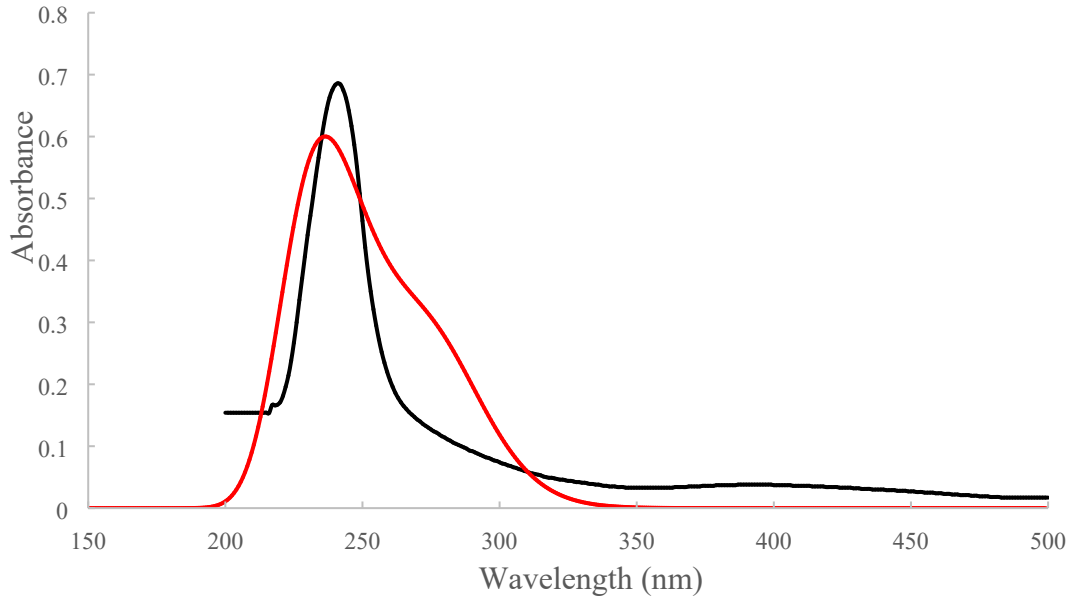

Figure S48: Simulated (red) and experimental (black)UV-vis spectra of **2b.**

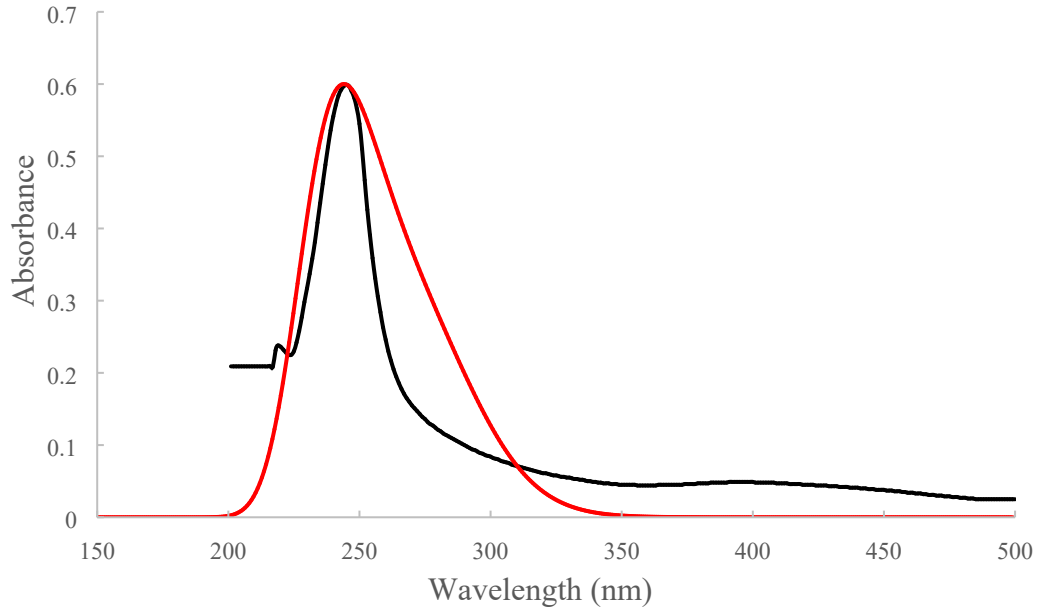

Figure S49: Simulated (red) and experimental (black)UV-vis spectra of **2c.**

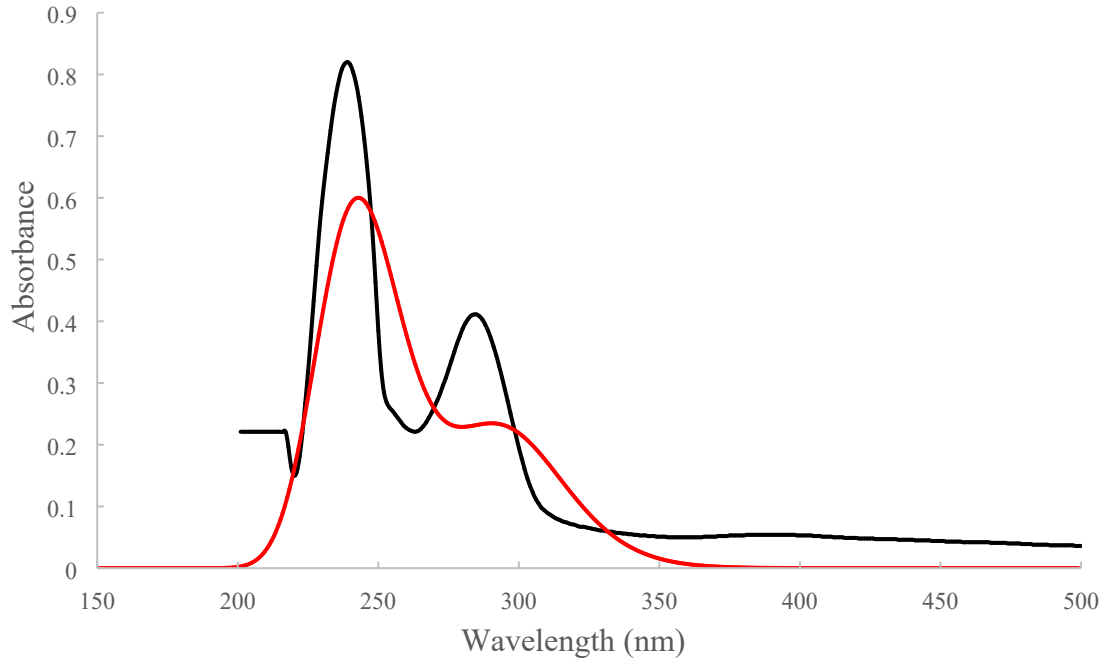

Figure S50: Simulated (red) and experimental (black)UV-vis spectra of **2d.**

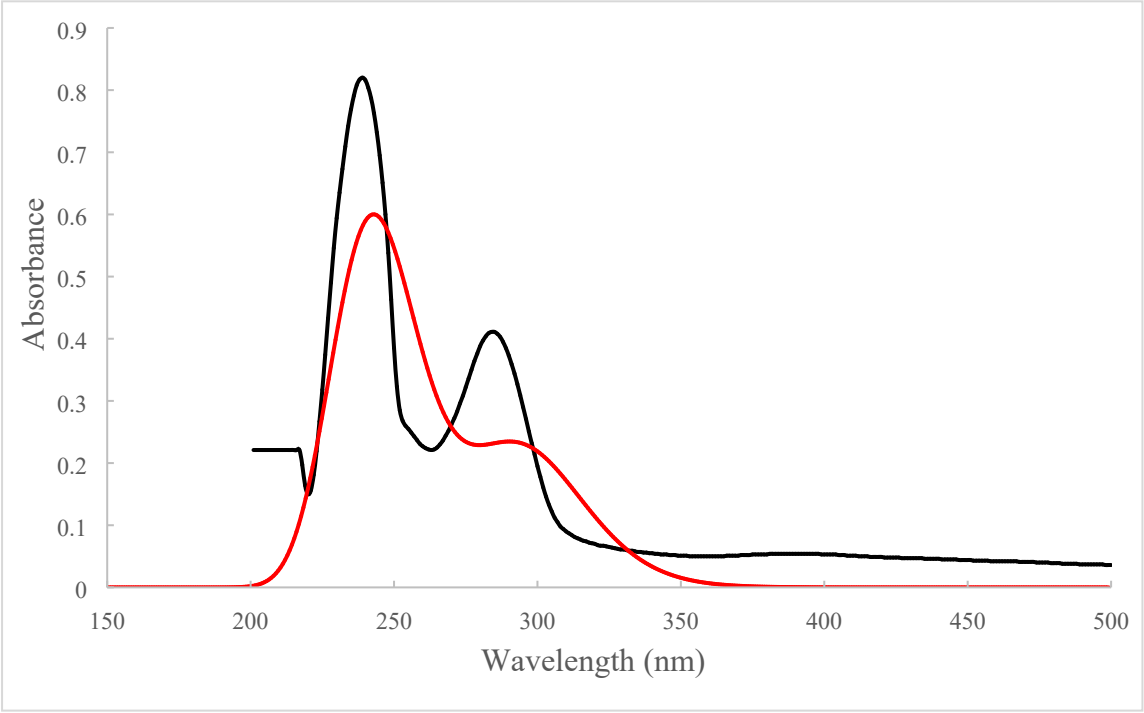

Figure S51: Simulated (red) and experimental (black)UV-vis spectra of **2e.**

Elemental analysis results

Table S1: Elemental results for compounds **1a-e** and **2a-e**.

Compound	Theoretical (%)			Found (%)		
	C	H	N	C	H	N
1a	54.88	7.12	23.27	54.79	7.03	23.15
1b	56.57	7.52	21.99	56.48	7.46	21.85
1c	64.45	6.68	17.68	64.37	6.53	17.62
1d	61.96	6.59	19.27	61.86	6.44	19.09
1e	63.04	6.94	18.38	62.94	6.81	18.24
2a	38.01	4.63	16.12	37.89	4.58	16.08
2b	39.86	5.02	15.49	39.81	4.90	15.38
2c	48.19	4.76	13.22	48.10	4.68	13.13
2d	45.31	4.56	14.09	45.23	4.47	13.89
2e	46.68	4.90	13.61	46.79	5.03	13.51

***In vitro* antibacterial testing results**

Experimental conditions:

Seven compounds were provided for antibacterial testing. **1e**, **2c**, and **2e** were diluted in 5% DMSO. **2b**, **2a**, and **2d** were diluted in 10% DMSO.

Bacterial strains selected:

- *Staphylococcus aureus* and *Enterococcus faecalis* (Gram positive)
- *Klebsiella pneumoniae* and *Pseudomonas aeruginosa* (Gram negative)

All bacterial strains were grown in Mueller Hinton Broth at pH 7.4 in a 30°C incubator for 24 hours

Statistical analysis:

All compounds were tested in triplicate on two separate occasions. Statistical analysis confirmed reproducibility of experimental data.

Results are depicted as the average percentage inhibition at each specified concentration (µg/ml). A range of values (% inhibition) are given to those values which show no significant difference ($p > 0.05$) between concentrations.

Table S2: Data showing

Test compound	Bacterial sp.		Test samples					Neomycin (control)				
			Concentration (µg/ml)									
			200	**100**	**50**	**25**	**12.5**	**200**	**100**	**50**	**25**	**12.5**
1a	*S. aureus*	mean	15.12	13.60	16.08	4.14	4.68	44.19	45.17	46.50	50.84	50.48
		SD	7.55	11.79	11.93	14.00	11.58	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	2.52	1.07	1.99	2.30	2.80	44.41	44.45	46.30	45.84	38.96
		SD	2.18	2.12	2.68	2.22	2.11	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	13.56	17.41	11.88	17.34	9.47	89.02	88.35	56.98	41.27	14.36
			4.07	2.63	13.85	3.33	7.61	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	19.55	23.59	24.72	18.86	9.90	63.07	68.62	68.58	65.38	43.45
			7.14	4.20	3.37	8.31	6.13	7.32	7.13	10.03	5.26	4.59
1b	*S. aureus*	mean	17.94	13.01	6.56	-0.04	12.06	44.18	45.17	46.50	50.84	50.48
			12.81	12.78	5.69	11.17	13.78	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	4.53	4.30	2.91	2.45	3.56	44.41	44.45	46.30	45.84	38.96
			1.36	1.66	2.47	2.09	2.18	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	3.70	2.47	3.60	-1.64	1.40	89.02	88.35	56.98	41.27	14.36
			6.80	5.82	8.35	8.64	13.39	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	0.53	2.59	7.39	9.34	0.36	63.07	68.62	68.58	65.38	43.45
			6.27	7.93	7.52	6.33	7.21	7.32	7.13	10.03	5.26	4.59
1c	*S. aureus*	mean	10.67	16.80	19.57	19.73	5.37	44.18	45.17	46.50	50.84	50.48
			3.92	9.52	7.03	9.84	6.18	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	4.46	2.87	1.66	2.28	2.55	44.41	44.45	46.30	45.84	38.96
			8.68	9.31	8.74	7.33	7.86	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	28.56	18.52	13.15	14.94	6.32	89.02	88.35	56.98	41.27	14.36
			3.67	2.41	3.39	3.72	4.04	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	3.06	10.26	8.04	6.76	1.75	63.07	68.62	68.58	65.38	43.45
			8.54	2.99	4.68	3.33	4.17	7.32	7.13	10.03	5.26	4.59
1d	*S. aureus*	mean	24.29	17.28	16.87	11.40	6.56	44.18	45.17	46.50	50.84	50.48
			9.30	5.68	5.35	3.97	3.64	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	3.38	3.51	3.33	2.22	2.23	44.41	44.45	46.30	45.84	38.96
			3.63	3.35	4.83	4.19	4.41	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	23.26	17.91	15.29	14.52	10.63	89.02	88.35	56.98	41.27	14.36
			4.55	2.61	4.31	3.91	3.50	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	1.67	6.10	3.74	4.95	-2.44	63.07	68.62	68.58	65.38	43.45

			1.87	5.95	5.23	3.11	3.72	7.32	7.13	10.03	5.26	4.59
1e	*S. aureus*	mean	18.06	20.27	31.04	31.43	39.77	44.18	45.17	46.50	50.84	50.48
		SD	5.54	2.75	4.76	6.81	6.96	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	7.04	4.28	5.12	3.92	2.64	44.41	44.45	46.30	45.84	38.96
		SD	3.67	1.68	1.09	2.17	2.09	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	5.70	3.51	6.57	5.06	3.92	89.02	88.35	56.98	41.27	14.36
		SD	2.68	2.80	1.91	1.90	2.41	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	29.88	27.76	28.68	23.87	14.46	63.07	68.62	68.58	65.38	43.45
		SD	5.85	5.73	7.82	2.90	8.18	7.32	7.13	10.03	5.26	4.59
2a	*S. aureus*	mean	61.04	59.26	24.06	27.80	45.02	44.18	45.17	46.50	50.84	50.48
		SD	5.46	8.44	7.23	6.65	6.08	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	85.46	88.71	54.09	18.99	12.56	44.41	44.45	46.30	45.84	38.96
		SD	5.49	3.56	5.66	2.02	4.38	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	84.67	82.75	25.53	26.56	15.19	89.02	88.35	56.98	41.27	14.36
		SD	8.67	10.63	5.22	6.50	5.46	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	81.32	68.47	51.02	34.08	42.70	63.07	68.62	68.58	65.38	43.45
		SD	8.55	4.43	4.70	9.00	5.75	7.32	7.13	10.03	5.26	4.59
2b	*S. aureus*	mean	44.28	56.81	59.01	18.94	27.88	44.18	45.17	46.50	50.84	50.48
		SD	9.26	4.99	2.23	7.63	5.75	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	81.34	86.39	82.60	26.41	11.26	44.41	44.45	46.30	45.84	38.96
		SD	5.37	4.35	7.91	7.65	2.97	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	85.60	89.91	91.08	36.52	12.98	89.02	88.35	56.98	41.27	14.36
		SD	3.61	3.33	0.57	4.55	4.85	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	91.02	72.71	59.03	21.27	12.20	63.07	68.62	68.58	65.38	43.45
		SD	1.13	2.63	4.79	6.03	3.14	7.32	7.13	10.03	5.26	4.59
2c	*S. aureus*	mean	60.77	64.02	46.85	11.36	10.78	44.18	45.17	46.50	50.84	50.48
		SD	4.85	3.10	6.49	6.16	8.33	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	83.97	82.71	84.12	76.28	15.83	44.41	44.45	46.30	45.84	38.96
		SD	5.49	4.43	7.06	6.96	1.65	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	93.02	97.46	91.74	91.80	27.01	89.02	88.35	56.98	41.27	14.36
		SD	1.80	2.27	10.83	10.50	8.98	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	86.71	85.43	83.23	70.74	46.60	63.07	68.62	68.58	65.38	43.45
		SD	2.12	8.00	7.74	6.15	8.22	7.32	7.13	10.03	5.26	4.59

2d	*S. aureus*	mean	59.53	47.40	14.79	30.71	31.55	44.18	45.17	46.50	50.84	50.48
		SD	3.87	6.60	5.25	5.86	4.89	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	80.16	84.23	32.17	13.24	9.00	44.41	44.45	46.30	45.84	38.96
		SD	6.57	6.23	9.62	2.08	5.89	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	90.00	85.79	34.73	25.76	14.14	89.02	88.35	56.98	41.27	14.36
		SD	1.87	6.74	4.57	4.99	2.59	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	73.69	38.73	25.68	23.98	19.93	63.07	68.62	68.58	65.38	43.45
		SD	3.92	3.67	3.72	6.91	4.07	7.32	7.13	10.03	5.26	4.59
2e	*S. aureus*	mean	51.61	55.65	11.77	8.17	15.04	44.18	45.17	46.50	50.84	50.48
		SD	5.56	6.31	9.51	5.25	9.85	3.84	2.13	2.37	5.70	4.66
	P. aeruginosa	mean	96.53	88.51	39.93	41.69	14.98	44.41	44.45	46.30	45.84	38.96
		SD	7.51	12.13	4.10	9.26	7.53	9.37	8.48	6.69	7.49	9.87
	K. pneumoniae	mean	88.79	90.11	89.97	49.08	21.24	89.02	88.35	56.98	41.27	14.36
		SD	1.48	3.11	1.03	5.39	8.59	1.79	0.81	31.98	13.63	6.57
	E. faecalis	mean	90.72	88.41	57.35	21.34	11.59	63.07	68.62	68.58	65.38	43.45
		SD	0.92	3.63	3.91	5.48	6.72	7.32	7.13	10.03	5.26	4.59

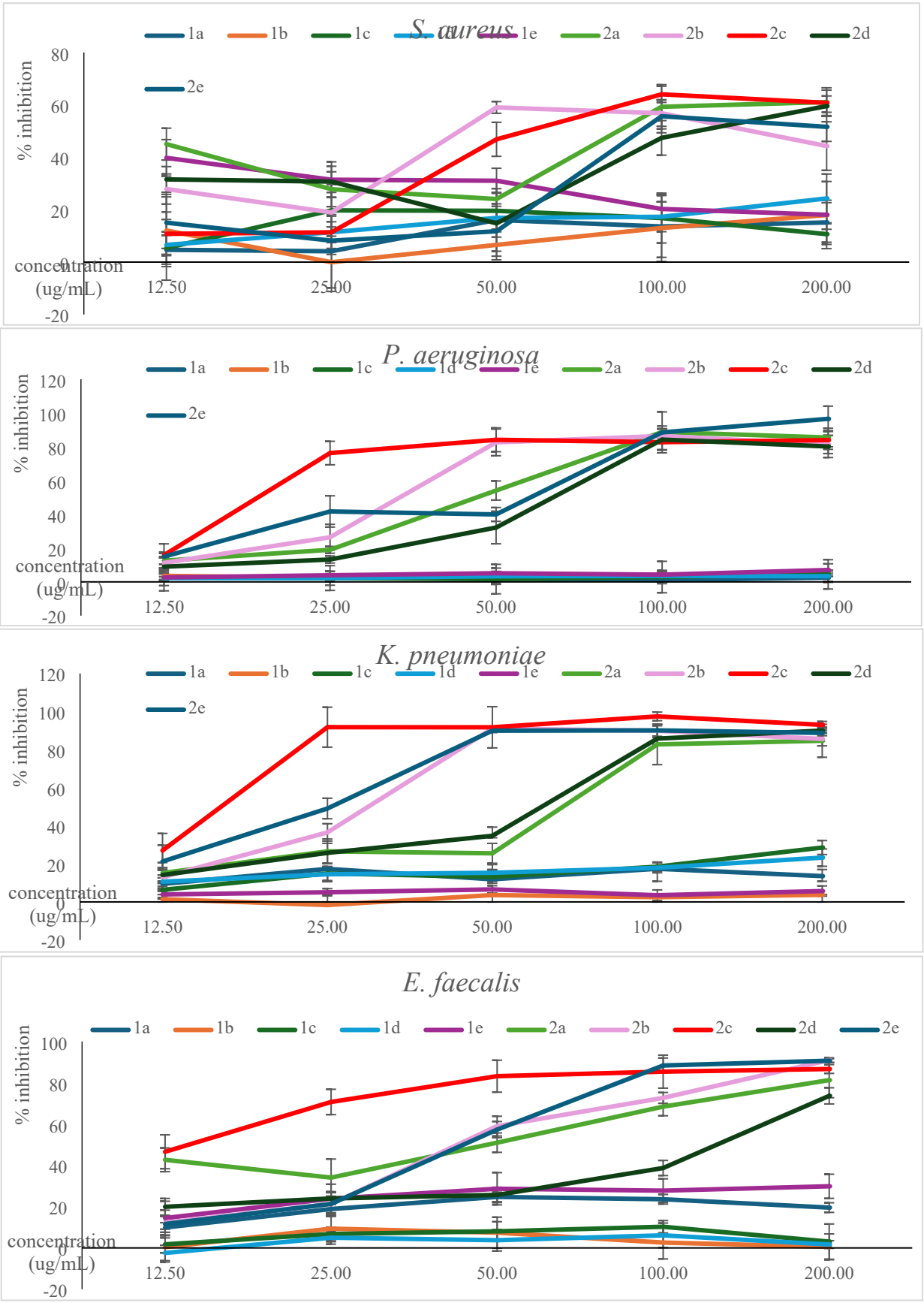

Figure S52: Graphs showing % inhibition vs concentration of various compounds tested against Gram-positive (*E. faecalis* and *S. aureus*) and Gram-negative (*P. aeruginosa* and *K. pnuemoniae*) bacteria.

Frontier molecular orbitals

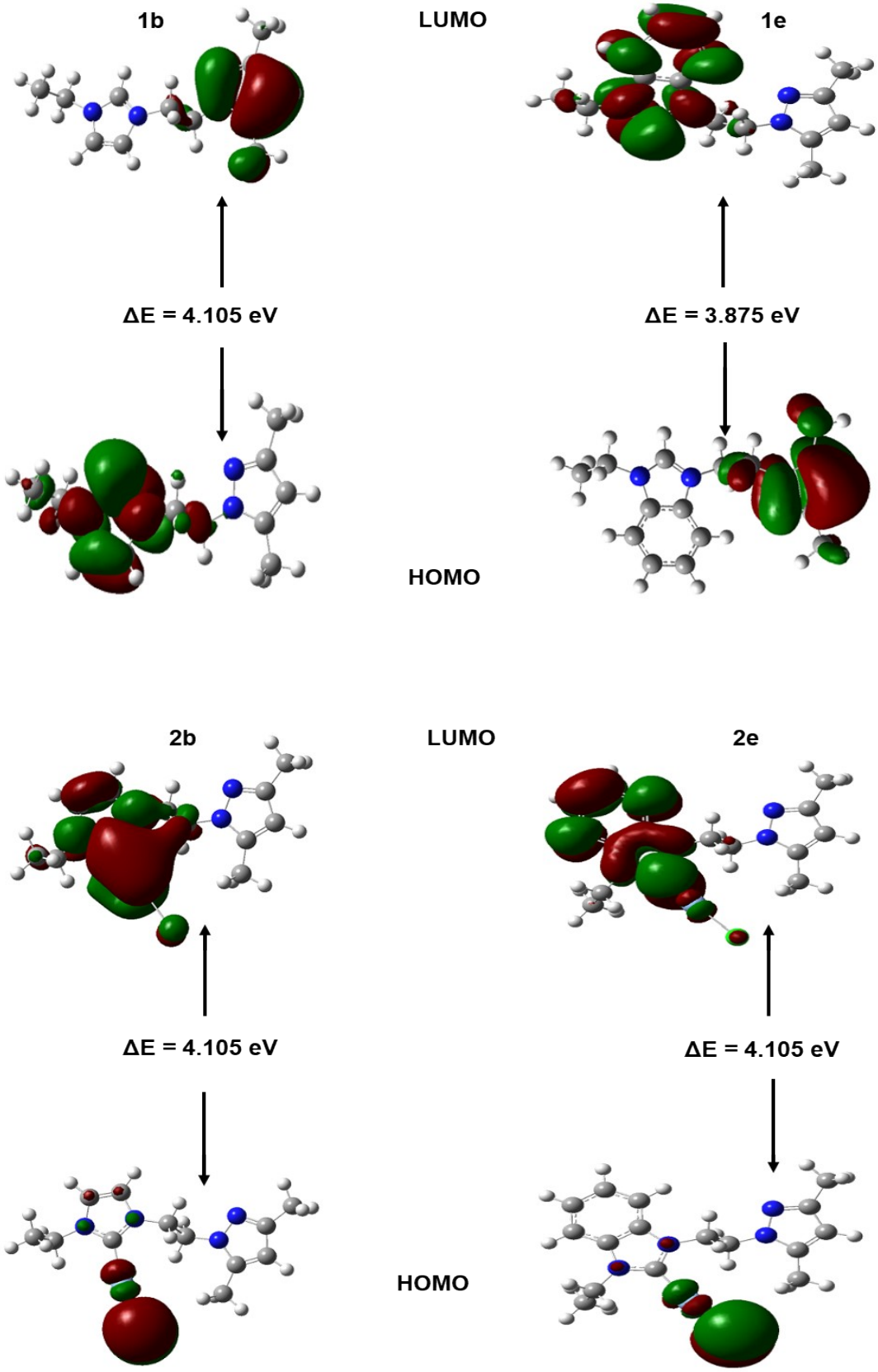

Figure S53: FMOs of **1b**, **1e**, **2b** and **2e**.

XYZ coordinates for the optimized compounds

Compound 1a E(B3LYP) = -648.227920 a.u. ZPVE = 173.25052 kcal/mol NImag = 0			**Compound 1b** E(B3LYP) = -687.550248 a.u. ZPVE = 191.13029 kcal/mol NImag = 0		
C	-4.01478800	-0.89880200	0.15335100	C	-3.52586000	-1.26160000	0.08282300
C	-2.78040000	-1.31098700	0.56512900	C	-2.27535000	-1.56884600	0.53619900
C	-2.64323800	0.82887300	0.03953900	C	-2.27911400	0.55263300	-0.07388800
H	-2.44072500	-2.27497200	0.91026800	H	-1.87483500	-2.49306500	0.92238600
H	-2.25247900	1.82255000	-0.12165400	H	-1.95490000	1.56386500	-0.26993200
H	-4.94668800	-1.43625500	0.07175600	H	-4.41281600	-1.87005400	0.00124100
N	-1.93750700	-0.21686700	0.49069400	N	-1.51065100	-0.42084000	0.43466200
C	-5.00271200	1.29853500	-0.65310100	N	-3.50751900	0.06828400	-0.29656300
H	-4.61364200	2.29983100	-0.83590300	C	-0.07745900	-0.28430100	0.75729500
H	-5.40194700	0.88866200	-1.58233900	C	0.82564100	-0.74824000	-0.40470700
H	-5.78738700	1.34562800	0.10396600	H	0.11592400	-0.85022700	1.67095200
N	-3.90800400	0.44155100	-0.17173800	H	0.12453500	0.76963900	0.95419900
C	-0.49259300	-0.19391700	0.79100300	H	0.84867700	-1.83760900	-0.48029600
C	0.35599300	-0.68034200	-0.40268900	H	0.43528600	-0.34800800	-1.34954700
H	-0.32592400	-0.80276500	1.68202100	C	4.33423600	0.01650100	-0.00890000
H	-0.21286800	0.83589600	1.01817800	H	5.39876400	-0.15625500	0.05936200
H	0.30600000	-1.76603800	-0.51095100	N	2.16634300	-0.26345000	-0.18496600
H	-0.02458200	-0.22639800	-1.32706500	N	2.34007500	1.08847500	-0.08307100
C	3.91346100	-0.15708200	-0.05503200	C	3.35576500	-0.94841300	-0.15263100
H	4.96551400	-0.40023100	-0.01298200	C	3.46168100	-2.43702800	-0.26764600
N	1.72916600	-0.29074300	-0.19567500	H	3.07407300	-2.80613400	-1.22466200
N	1.99254600	1.04356500	-0.05815900	H	4.51117100	-2.73097700	-0.20514700
C	2.87184300	-1.05196200	-0.20694400	H	2.92854700	-2.95626800	0.53778300
C	2.87820800	-2.54010800	-0.36740900	C	3.65652000	1.26435500	0.02979400
H	2.45025800	-2.85399200	-1.32693500	C	4.24093900	2.63538900	0.17520000
H	3.90719000	-2.90318900	-0.33445000	H	4.95178100	2.84698900	-0.63053800
H	2.32694200	-3.04805200	0.43299400	H	3.45065000	3.38888100	0.14530700
C	3.31946800	1.13035500	0.03334200	H	4.78088800	2.73620300	1.12288600
C	3.99489400	2.45551800	0.20670400	C	-4.66300900	0.84231100	-0.81273200
H	4.70587400	2.64316100	-0.60479100	C	-5.66218500	1.19945100	0.28561600
H	3.25563700	3.25966300	0.21116900	H	-5.12386700	0.23541400	-1.59617400
H	4.55459000	2.49345900	1.14750900	H	-4.25263800	1.73691600	-1.28638900
				H	-6.48507800	1.76900500	-0.15508500
				H	-6.08589100	0.30605300	0.75292000
				H	-5.19883900	1.81508500	1.06175400

Compound 1c			**Compound 1d**		
E(B3LYP) = -879.297581 a.u.			E(B3LYP) = -801.888137 a.u.		
ZPVE = 224.32130 kcal/mol			ZPVE = 202.96894 kcal/mol		
NImag = 0			NImag = 0		
C	1.90651100	-1.25842200	-0.05967600	C	3.34099800	-2.44932500	0.58940400
C	0.66724900	-1.49677500	-0.58071100	C	3.94614700	-1.20770800	0.41954800
C	0.66227800	0.53115300	0.29014500	C	3.10346200	-0.15288500	0.05773800
H	0.27734200	-2.35805700	-1.10014000	C	1.72214300	-0.34015400	-0.12438000
H	0.33723600	1.51246400	0.60198900	C	1.10987400	-1.58597100	0.04697200
H	2.79727800	-1.86571500	-0.04747300	C	1.95239200	-2.63349000	0.40719100
N	-0.09640200	-0.36517900	-0.35701500	H	3.95293400	-3.29998100	0.87021300
N	1.88231900	0.01369200	0.48020800	H	5.01277700	-1.07346000	0.56033100
C	-1.51386600	-0.17273000	-0.71491000	H	0.03881700	-1.71752900	-0.08298500
C	-2.46438500	-0.78395900	0.33529800	H	1.52990200	-3.62177500	0.55451600
H	-1.67306200	-0.60698800	-1.70420900	N	3.36057300	1.19726200	-0.20012800
H	-1.70483600	0.89981100	-0.77403900	N	1.19608300	0.90608200	-0.48685100
H	-2.48193600	-1.87402200	0.26868400	C	4.67267400	1.84759600	-0.14219600
H	-2.11981300	-0.50835700	1.34043600	H	5.34747700	1.37508100	-0.85930000
C	-5.95844700	0.01424000	-0.12219500	H	5.08163200	1.75799000	0.86650800
H	-7.01680400	-0.15205900	-0.26347800	C	-0.21919900	1.17568600	-0.78614500
N	-3.79857500	-0.27861200	0.12014500	H	-0.56238300	0.38741400	-1.45906000
N	-3.98065000	1.07416300	0.18764300	H	-0.27063800	2.12953100	-1.31503300
C	-4.97806800	-0.95753300	-0.05924100	C	-1.10378400	1.16588200	0.48875400
C	-5.07447800	-2.44875900	-0.14563500	H	-1.29737500	2.18172900	0.83767500
H	-4.72715200	-2.93910100	0.77158000	H	-0.58280100	0.63138500	1.29155300
H	-6.11708000	-2.73594500	-0.29490800	C	-4.47229400	-0.07135200	0.04020500
H	-4.49996100	-2.85548600	-0.98651600	H	-5.55278800	-0.06296700	0.03388900
C	-5.29198600	1.25866400	0.03561100	C	-3.61501800	-1.15599800	-0.27910900
C	-5.88208900	2.63500500	0.04339700	C	-3.99026000	-2.54390700	-0.69836500
H	-6.63253100	2.73647200	0.83450900	H	-4.59127100	-3.03856200	0.07203400
H	-5.10128500	3.38043200	0.21043100	H	-4.58426700	-2.53109800	-1.61841500
H	-6.37711500	2.85817600	-0.90792200	H	-3.09459800	-3.14402000	-0.87482100
C	3.00644200	0.68777600	1.19965700	C	-3.64621900	0.98939100	0.36321600
H	3.02125300	0.29014600	2.21795100	C	-3.97492500	2.38504800	0.79282200
H	2.73802400	1.74598200	1.24944700	H	-3.60611900	2.60339600	1.80199200
C	4.33557800	0.47921800	0.51624900	H	-3.56364500	3.13847100	0.11065000
C	4.65205700	1.18351800	-0.65529100	H	-5.05885300	2.51400300	0.80554900
C	5.26837000	-0.41638500	1.05584600	N	-2.36672800	0.51617900	0.22469700
C	5.88097800	0.98365500	-1.28404500	N	-2.33587800	-0.79427600	-0.16120900
H	3.94382300	1.89555700	-1.07267600	C	2.20181000	1.78724200	-0.51908900
C	6.50110600	-0.61371500	0.42691100	H	4.55958800	2.90216400	-0.39360500
H	5.04177400	-0.94919900	1.97639900	H	2.09645600	2.83115500	-0.77663900
C	6.80599000	0.08336200	-0.74399700				
H	6.12224000	1.53628500	-2.18656800				
H	7.22146300	-1.30320300	0.85557500				
H	7.76487000	-0.06552100	-1.23044200				

Compound 1e E(B3LYP) = -841.209467 a.u. ZPVE = 220.80820 kcal/mol NImag = 0			**Compound 2a** E(B3LYP) = -1253.857644 a.u. ZPVE = 166.48615 kcal/mol NImag = 0		
C	2.85384800	-2.73781400	0.69549600	C	0.50011500	4.19769300	-4.48600600
C	3.53329600	-1.52691000	0.60757000	C	-0.66414900	6.00536100	-3.20859900
C	2.77144400	-0.41044500	0.24859200	H	-1.04905300	6.88974100	-3.72375700
C	1.39253900	-0.51420200	-0.00666300	H	0.35067700	6.20291300	-2.86345100
C	0.70497000	-1.72930000	0.08201400	C	0.92164200	2.23750800	-5.98609200
C	1.46861700	-2.83676800	0.43702600	H	1.88111200	2.69607300	-6.22329400
H	3.40358500	-3.63161300	0.97098400	H	0.45256300	1.93259100	-6.92489700
H	4.59674100	-1.46141900	0.80738200	C	1.12457000	1.01827300	-5.07125200
H	-0.36404800	-1.79425500	-0.10284400	H	0.15629000	0.64225600	-4.72976000
H	0.98585400	-3.80460100	0.52147900	H	1.70259600	1.31847700	-4.18808300
N	3.11092100	0.93570400	0.07222200	N	1.80057100	-0.05226200	-5.78166300
N	0.94971500	0.77348700	-0.33134600	C	2.57556900	-1.99048600	-6.46360100
C	-0.43527500	1.13383300	-0.67134900	H	2.71637700	-3.04988500	-6.62684100
H	-0.79355800	0.39551200	-1.39141300	C	3.33944600	-0.92018400	-6.99641400
H	-0.41469700	2.11089900	-1.15838100	C	1.59664500	-1.40208700	-5.68020900
C	-1.36973200	1.11830400	0.56713700	N	2.86683600	0.25198100	-6.57148100
H	-1.51146600	2.12558400	0.96275200	N	0.06308400	3.24093500	-5.35023700
H	-0.91775900	0.50953300	1.35871400	N	-0.62772900	4.86648800	-4.12389500
C	-4.78951400	0.13251100	-0.07572000	Ag	2.47576900	4.55918700	-3.80037800
H	-5.86597900	0.21331700	-0.12354800	Cl	4.63777900	5.00570000	-2.94933100
C	-3.99140300	-0.98988100	-0.41722000	C	0.51162300	-2.01758900	-4.85147900
C	-4.43725400	-2.32750100	-0.92211400	H	-0.48783600	-1.69503400	-5.16848900
H	-5.10054400	-2.81862400	-0.20219300	H	0.61802500	-1.77645800	-3.78696900
H	-4.99010700	-2.23010600	-1.86254100	C	4.52296000	-0.97855800	-7.91446700
H	-3.57528700	-2.97613500	-1.09465700	H	5.33385200	-1.57223800	-7.47776000
C	-3.91086800	1.11846200	0.33408300	H	4.89854800	0.03017000	-8.10246500
C	-4.16634700	2.51020600	0.82220000	H	0.55222300	-3.10480100	-4.94975200
H	-3.82544900	2.65428900	1.85425500	H	4.26139400	-1.43597900	-8.87576500
H	-3.68009900	3.26704800	0.19533600	C	-1.74910400	4.33961200	-4.74870900
H	-5.23937300	2.70993100	0.80112200	H	-2.73945000	4.74149100	-4.60141200
N	-2.66006900	0.56819100	0.22134200	C	-1.31303900	3.31008200	-5.52162400
N	-2.69771300	-0.72065000	-0.23075500	H	-1.85084400	2.64299900	-6.17734100
C	2.00069000	1.59936700	-0.27146200	H	-1.29974100	5.77599500	-2.34897000
H	1.96047200	2.65906300	-0.47828300				
C	4.46272000	1.52304700	0.18595000				
C	5.32894700	1.25256600	-1.04398100				
H	4.91114100	1.11030500	1.09352700				
H	4.32892100	2.59532300	0.34878300				
H	6.31496500	1.70063000	-0.89212600				
H	5.46688700	0.18170700	-1.21452500				
H	4.88974900	1.69363500	-1.94342000				

Compound 2b E(B3LYP) = -1293.177686 a.u. ZPVE = 184.39332 kcal/mol NImag = 0			**Compound 2c** E(B3LYP) = -1484.919256 a.u. ZPVE = 217.61171 kcal/mol NImag = 0		
C	0.31018700	4.00480700 -4.17681000	C	0.91321300	4.34819500 -4.95349600
C	0.60932600	2.07253400 -5.74091600	C	0.26092300	6.34255400 -3.57477800
H	1.41284800	2.64451100 -6.20408500	H	-0.54720500	6.99864800 -3.91314000
H	-0.03009100	1.68260700 -6.53700800	H	1.19292100	6.70485800 -4.01561000
C	1.19026400	0.91611500 -4.90991800	C	0.86815800	2.10563200 -6.06704200
H	0.39345900	0.42297900 -4.34674000	H	1.46598800	2.55378800 -6.86025200
H	1.91762100	1.31422700 -4.19138700	H	0.04992100	1.55055300 -6.53304100
N	1.81548200	-0.07302900 -5.76894300	C	1.73537900	1.16188700 -5.21668100
C	2.63814600	-1.91092200 -6.64523600	H	1.16861900	0.81206300 -4.34981900
H	2.86015200	-2.94745000 -6.85767100	H	2.61438100	1.70702400 -4.85067000
C	3.13914500	-0.76125200 -7.30880600	N	2.14447900	0.00200600 -5.98742300
C	1.79395900	-1.43703600 -5.65475200	C	2.77480700	-1.99319400 -6.65398800
N	2.64019700	0.34972500 -6.76600600	H	2.97729400	-3.05427600 -6.69767500
N	-0.19289200	2.97373900 -4.90939700	C	3.01545500	-1.02050700 -7.65854300
N	-0.76972000	4.52263500 -3.53274800	C	2.21975900	-1.30519300 -5.58776000
Ag	2.31802100	4.67166400 -4.01831900	N	2.63625200	0.18832000 -7.24296700
Cl	4.52776300	5.47506700 -3.74781800	N	0.28921400	3.17549300 -5.25043000
C	0.99450000	-2.17184000 -4.62321100	N	0.03465000	5.00433600 -4.14810800
H	-0.08049700	-1.97054100 -4.70853200	Ag	2.84910600	5.00117600 -5.52389800
H	1.30208100	-1.91522900 -3.60233800	Cl	5.02418500	5.77789800 -6.03450600
C	4.09171600	-0.68531600 -8.46369800	C	1.77570600	-1.78989700 -4.24197900
H	5.04105300	-1.17878400 -8.22708100	H	0.71166300	-1.59523800 -4.05955200
H	4.29896400	0.35950200 -8.70728300	H	2.34431700	-1.32561000 -3.42726200
H	1.13813400	-3.24719100 -4.75108100	C	3.60261100	-1.20856500 -9.02485600
H	3.68015200	-1.17405600 -9.35448200	H	4.60267300	-1.65291000 -8.96842600
C	-1.92822900	3.83187500 -3.85832700	H	3.68340000	-0.24375000 -9.53134400
H	-2.89486600	4.09543100 -3.45818300	C	0.33748900	6.33456200 -2.06132500
C	-1.56363700	2.84899200 -4.72371000	C	1.41994700	5.72472100 -1.40893900
H	-2.15019300	2.09105500 -5.21934600	C	-0.66136000	6.94838400 -1.29575500
C	-0.73073400	5.70472800 -2.65915700	C	1.49524700	5.72543900 -0.01566200
C	-1.13625000	6.98777900 -3.38549300	H	2.20876700	5.25873700 -1.99388600
H	0.29028200	5.78040100 -2.27898200	C	-0.58737200	6.95030200 0.10137700
H	-1.39087900	5.50663800 -1.80856800	H	-1.49702800	7.43735700 -1.79171400
H	-1.08911100	7.83322300 -2.69191700	C	0.48995000	6.33613500 0.74311900
H	-0.45774000	7.19112200 -4.21895500	H	2.34185900	5.25757300 0.47834800
H	-2.15743900	6.92375300 -3.77538400	H	-1.36711600	7.43332500 0.68320500
			H	0.55224000	6.33914400 1.82747000
			H	1.92753400	-2.86977000 -4.17719400
			H	2.98229300	-1.87178000 -9.63893900
			C	-1.11535700	4.25645400 -3.94072400
			H	-1.93146800	4.60431200 -3.32750600
			C	-0.95473300	3.10053200 -4.63654000
			H	-1.61166600	2.25324800 -4.75834000

Compound 2d			**Compound 2e**		
E(B3LYP) = -1407.519177 a.u.			E(B3LYP) = -1446.833001 a.u.		
ZPVE = 196.17235 kcal/mol			ZPVE = 213.89093 kcal/mol		
NImag = 0			NImag = 0		
C	-1.53781900	-0.09121500	2.30842500	C	-3.33676400	1.09457900	-3.45653200
C	-0.59111300	-0.39703900	1.32969100	C	-2.15721800	1.14962100	-4.20033400
C	-0.53605000	0.44569200	0.21743200	C	-1.36928900	2.29474200	-4.06043900
C	-1.39541400	1.54820400	0.08570100	C	-1.74829600	3.34693000	-3.21125000
C	-2.34260500	1.85689200	1.06478800	C	-2.93019000	3.29366000	-2.46809500
C	-2.39755200	1.01673300	2.17778700	C	-3.71678600	2.14916300	-2.60442300
H	-1.61249900	-0.72024400	3.18984900	H	-3.97579200	0.22103700	-3.53878700
H	0.07009600	-1.25087100	1.43349100	H	-1.87370100	0.33668800	-4.86046900
H	-3.00363000	2.71222300	0.97264800	H	-3.22965900	4.10347400	-1.81149300
H	-3.11932000	1.22363600	2.96159100	H	-4.64208800	2.07103200	-2.04238200
N	0.26695300	0.44140600	-0.92425500	C	0.20932100	3.92162900	-4.20673300
N	-1.06898600	2.14440300	-1.13505200	C	-0.73604100	5.59075700	-2.59903800
C	1.30269900	-0.54860900	-1.19215000	C	-0.20638400	5.44460800	-1.17122600
H	0.86469000	-1.55020400	-1.23931700	H	-1.75573400	5.98988100	-2.60478000
H	2.06357500	-0.52147600	-0.40631900	H	-0.11031500	6.27645900	-3.17453300
C	-1.69837900	3.34906800	-1.67621600	H	-0.22612700	6.41802600	-0.67106800
H	-2.73163300	3.39257000	-1.32573700	H	-0.81172400	4.74690700	-0.58410000
H	-1.71197100	3.26232800	-2.76503000	H	0.82724100	5.08665200	-1.17844500
C	-0.95504200	4.62949200	-1.25113800	C	0.59913600	1.87726800	-5.59559400
H	0.05580400	4.63013300	-1.66522600	H	1.16418500	2.54347100	-6.24678200
H	-0.88080600	4.67636800	-0.15985800	H	-0.10166200	1.31656600	-6.21981700
C	-2.36325400	7.57516300	-2.80796900	C	1.55002200	0.91609500	-4.86106700
H	-2.44186500	8.40304200	-3.49862800	H	1.00269100	0.35439900	-4.09960900
C	-3.27412000	7.20886100	-1.78412500	H	2.33239700	1.49718600	-4.35648400
C	-4.56507600	7.86778500	-1.40088500	N	2.14150500	-0.03450600	-5.78482200
H	-4.40518900	8.90727400	-1.09213300	C	3.07973500	-1.78446400	-6.72286500
H	-5.27043100	7.88030300	-2.23975000	H	3.44130900	-2.78392700	-6.92075600
H	-5.02719400	7.32958300	-0.56935700	C	3.18831800	-0.64044000	-7.55514600
C	-1.33107400	6.65274900	-2.74716500	C	3.82105200	-0.52179200	-8.90885000
C	-0.08194400	6.52952900	-3.56455100	H	3.76695700	0.51295300	-9.25568200
H	0.82056600	6.63724900	-2.95091900	H	4.87467100	-0.82156900	-8.88129400
H	-0.00830700	5.57175500	-4.09220900	H	3.31666700	-1.16037600	-9.64339800
H	-0.06301000	7.32005900	-4.31796600	C	2.40760400	-1.36284900	-5.58762200
N	-1.65403000	5.80723700	-1.71931300	C	2.01940700	-2.11293300	-4.35074100
N	-2.83913700	6.13155900	-1.12850900	H	0.93565900	-2.10500900	-4.18130200
C	-0.05392300	1.47476600	-1.74624200	H	2.32919300	-3.15610700	-4.44665100
Ag	0.84633300	2.07178800	-3.56893800	H	2.49965800	-1.70547800	-3.45295100
Cl	1.79401600	2.94684700	-5.55171700	N	2.62271700	0.41842000	-6.97486900
H	1.76586300	-0.31234400	-2.15009800	N	-0.16580200	2.68992200	-4.65009100
				N	-0.75454300	4.31970800	-3.33393900
				Ag	1.95941700	5.00996500	-4.70657500
				Cl	3.89899600	6.28273900	-5.16389700