Supporting Information

Conformationally Constrained Analogues of Diacylglycerol. 30. An Investigation of Diacylglycerol-lactones Containing Heteroaryl Groups Reveals Compounds with High Selectivity for Ras Guanyl Nucleotide-Releasing Proteins

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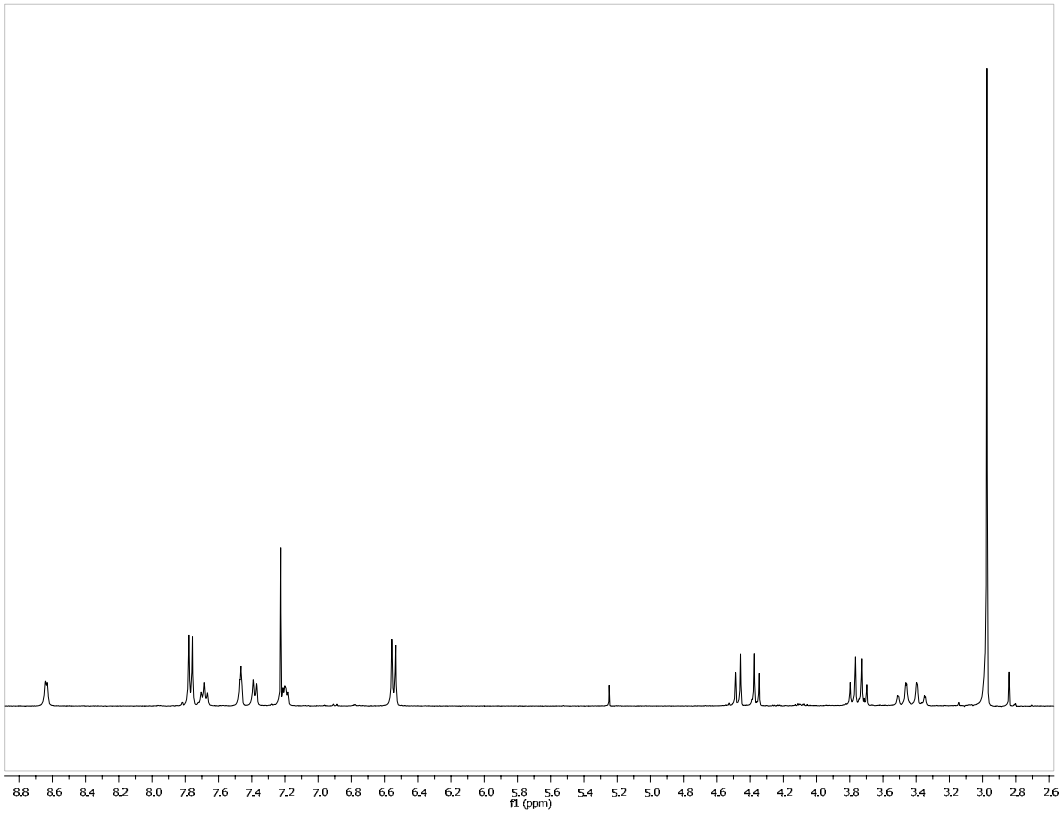
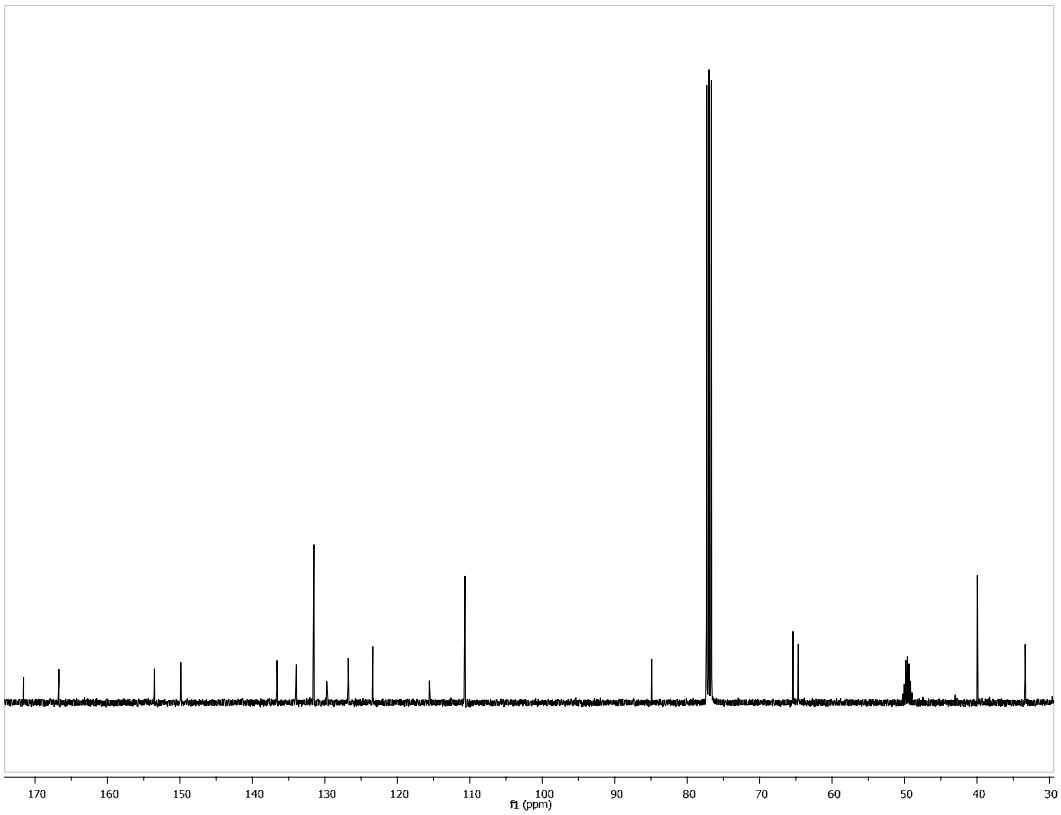
Table of Elemental Analysis

Compound Number	Formula	Calculated			Found		
		C	H	N	C	H	N
7-*E* (R_2 = 2-pyridyl)	$C_{26}H_{25}NO_5$	72.37	5.84	3.25	72.47	5.99	3.21
7-*E* (R_2 = 3-pyridyl)	$C_{26}H_{25}NO_5 \cdot 0.6H_2O$	70.60	5.97	3.17	70.21	5.94	2.96
7-*Z* (R_2 = 3-pyridyl)	$C_{26}H_{25}NO_5 \cdot 0.3H_2O$	71.48	5.91	3.21	71.45	5.80	3.23
7-*E* (R_2 = 4-pyridyl)	$C_{26}H_{25}NO_5 \cdot 0.3H_2O$	71.48	5.91	3.21	71.34	5.73	3.30
7-*E* (R_2 = 2-quinolyl)	$C_{30}H_{27}NO_5$	74.83	5.65	2.91	74.54	5.72	2.89
7-*Z* (R_2 = 2-quinolyl)	$C_{30}H_{27}NO_5$	74.83	5.65	2.91	74.76	5.60	2.89
7-*Z* (R_2 = 3-quinolyl)	$C_{30}H_{27}NO_5$	74.83	5.65	2.91	74.76	5.60	2.89
9-*E* (R_2 = 2-pyridyl)	$C_{19}H_{19}NO_4$	70.14	5.89	4.31	70.00	6.02	4.03
9-*Z* (R_2 = 2-pyridyl)	$C_{19}H_{19}NO_4$	70.14	5.89	4.31	70.00	5.83	4.25
9-*E* (R_2 = 3-pyridyl)	$C_{19}H_{19}NO_4$	70.14	5.89	4.31	69.99	5.93	4.28
9-*Z* (R_2 = 3-pyridyl)	$C_{19}H_{19}NO_4 \cdot 0.2H_2O$	69.37	5.94	4.26	69.35	5.94	4.23
9-*E* (R_2 = 4-pyridyl)	$C_{19}H_{19}NO_4 \cdot 0.3H_2O$	68.99	5.97	4.23	68.96	5.77	4.18
9-*Z* (R_2 = 4-pyridyl)	$C_{19}H_{19}NO_4 \cdot 0.2H_2O$	69.37	5.94	4.26	69.23	5.86	4.18
9-*E* (R_2 = 3-quinolyl)	$C_{23}H_{21}NO_4 \cdot 0.3H_2O$	72.54	5.72	3.68	72.58	5.64	3.73
9-*Z* (R_2 = 3-quinolyl)	$C_{23}H_{21}NO_4 \cdot 0.8H_2O$	70.86	5.84	3.59	70.78	5.60	3.65
11-*E* (R_1 = 4-$(CH_3)_2NC_6H_4$-, R_2 = 2-pyridyl)	$C_{28}H_{28}N_2O_5$	71.17	5.97	5.93	71.22	5.96	5.89
11-*E* (R_1 = 4-$(CH_3)_2NC_6H_4$-, R_2 = 3-pyridyl)	$C_{28}H_{28}N_2O_5 \cdot 0.3H_2O$	70.36	6.03	5.86	70.31	5.95	5.73
11-*Z* (R_1 = 4-$(CH_3)_2NC_6H_4$-, R_2 = 3-pyridyl)	$C_{28}H_{28}N_2O_5 \cdot 0.1H_2O$	70.90	5.99	5.91	70.60	5.99	5.94
11-*E* (R_1 = 4-$(CH_3)_2NC_6H_4$-, R_2 = 4-pyridyl)	$C_{28}H_{28}N_2O_5 \cdot 0.5H_2O$	69.84	6.07	5.82	69.63	5.84	5.71
11-*Z* (R_1 = 4-$(CH_3)_2NC_6H_4$-, R_2 = 4-pyridyl)	$C_{28}H_{28}N_2O_5$	71.17	5.97	5.93	71.37	5.93	5.97
11-*E* (R_1 = 4-$(CH_3)_2NC_6H_4$-, R_2 = 2-quinolyl)	$C_{32}H_{30}N_2O_5 \cdot 0.1H_2O$	73.29	5.80	5.34	72.91	5.79	5.39
11-*E* (R_1 = 4-$(CH_3)_2NC_6H_4$-, R_2 = 3-quinolyl)	$C_{32}H_{30}N_2O_5 \cdot 0.5H_2O$	72.30	5.88	5.27	72.12	5.75	5.19
11-*E* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 2-pyridyl)	$C_{27}H_{25}NO_6$	70.58	5.48	3.05	70.45	5.50	2.91
11-*Z* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 2-pyridyl)	$C_{27}H_{25}NO_6 \cdot 0.5H_2O$	69.22	5.59	2.99	69.26	5.32	3.15
11-*E* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 3-pyridyl)	$C_{27}H_{25}NO_6$	70.58	5.48	3.05	70.52	5.45	2.96
11-*Z* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 3-pyridyl)	$C_{27}H_{25}NO_6 \cdot 0.5H_2O$	69.22	5.59	2.99	69.11	5.39	2.81
11-*E* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 4-pyridyl)	$C_{27}H_{25}NO_6$	70.58	5.48	3.05	70.60	5.65	3.10
11-*Z* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 4-pyridyl)	$C_{27}H_{25}NO_6$	70.58	5.48	3.05	70.15	5.40	2.99

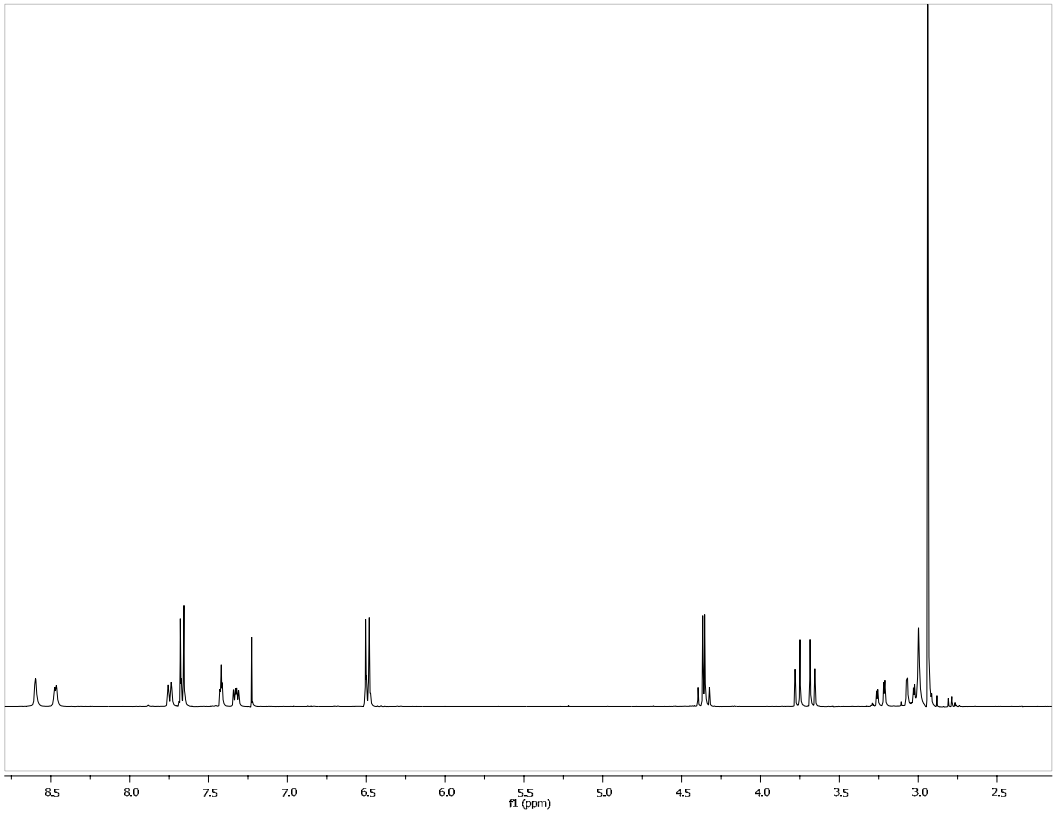
		Calculated			Found		
Compound Number	**Formula**	**C**	**H**	**N**	**C**	**H**	**N**
11-*E* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 2-quinolyl)	$C_{31}H_{27}NO_6$•0.1H_2O	72.81	5.36	2.74	72.48	5.34	2.70
11-*Z* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 2-quinolyl)	$C_{31}H_{27}NO_6$•0.2H_2O	72.56	5.38	2.73	72.27	5.32	2.78
11-*E* (R_1 = 4-$CH_3OC_6H_4$-, R_2 = 3-quinolyl)	$C_{31}H_{27}NO_6$•0.5H_2O	71.80	5.44	2.70	71.92	5.38	2.76
11-*E* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 2-pyridyl)	$C_{27}H_{33}NO_5$	71.82	7.37	3.10	71.87	7.44	3.06
11-*Z* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 2-pyridyl)	$C_{27}H_{33}NO_5$•0.6H_2O	70.14	7.46	3.03	69.97	7.22	3.03
11-*E* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 3-pyridyl)	$C_{27}H_{33}NO_5$	71.82	7.37	3.10	71.71	7.57	3.30
11-*Z* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 3-pyridyl)	$C_{27}H_{33}NO_5$	71.82	7.37	3.10	71.84	7.50	3.04
11-*E* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 4-pyridyl)	$C_{27}H_{33}NO_5$•H_2O	69.06	7.51	2.98	68.67	7.09	3.05
11-*Z* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 4-pyridyl)	$C_{27}H_{33}NO_5$•0.6H_2O	70.14	7.46	3.03	70.03	7.39	2.80
11-*E* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 2-quinolyl)	$C_{31}H_{35}NO_5$.•0.5H_2O	72.92	7.11	2.74	72.63	6.97	2.72
11-*Z* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 2-quinolyl)	$C_{31}H_{35}NO_5$•0.2H_2O	73.70	7.06	2.77	73.46	7.01	2.68
11-*Z* (R_1 = $CH(CH_2CH_2CH_3)_2$, R_2 = 3-quinolyl)	$C_{31}H_{35}NO_5$•0.2H_2O	73.70	7.06	2.77	73.48	7.07	2.78
11-*E* (R^1= $CH_2CH[CH_2CH(CH_3)_2]_2$, R^2= 2-pyridyl)	$C_{30}H_{39}NO_5$	72.99	7.96	2.84	73.04	8.07	2.90
12b-*E*	$C_{21}H_{22}N_2O_5$•0.1H_2O	65.96	5.80	7.33	65.96	5.85	7.26
12c-*E*	$C_{21}H_{22}N_2O_5$•0.9H_2O	63.27	6.02	7.03	63.01	5.62	6.89
12c-*Z*	$C_{21}H_{22}N_2O_5$•0.4H_2O	64.74	5.90	7.19	64.88	5.94	7.19
12d-*E*	$C_{25}H_{24}N_2O_5$•0.1H_2O	69.14	5.62	6.45	69.00	5.63	6.33
12d-*Z*	$C_{25}H_{24}N_2O_5$•0.1H_2O	69.14	5.62	6.45	68.99	5.60	6.33
12d-*E*	$C_{25}H_{24}N_2O_5$•0.8H_2O	67.19	5.77	6.27	66.99	5.43	6.15
12e-*Z*	$C_{25}H_{24}N_2O_5$•0.6H_2O	67.74	5.73	6.32	67.79	5.48	6.31
12f-*E*	$C_{25}H_{26}N_2O_5$•0.9H_2O	66.62	6.22	6.22	66.38	5.98	6.40
12g-*E*	$C_{20}H_{19}NO_6$•0.1H_2O	64.72	5.21	3.77	64.55	5.43	3.61
12g-*Z*	$C_{20}H_{19}NO_6$•0.1H_2O	64.72	5.21	3.77	64.55	5.34	3.61
12h-*E*	$C_{20}H_{19}NO_6$•0.1H_2O	64.72	5.21	3.77	64.59	5.11	3.76
12h-*Z*	$C_{20}H_{19}NO_6$	65.03	5.18	3.79	64.92	5.23	3.75
12i-*E*	$C_{20}H_{19}NO_6$•0.4H_2O	63.79	5.30	3.72	63.59	5.02	3.71
12i-*Z*	$C_{20}H_{19}NO_6$	65.03	5.18	3.79	64.77	5.22	3.70
12j-*E*	$C_{24}H_{21}NO_6$•H_2O	65.90	5.30	3.20	65.86	5.00	3.19
12j-*Z*	$C_{24}H_{21}NO_6$.0.5H_2O	67.28	5.18	3.27	67.12	4.99	3.26

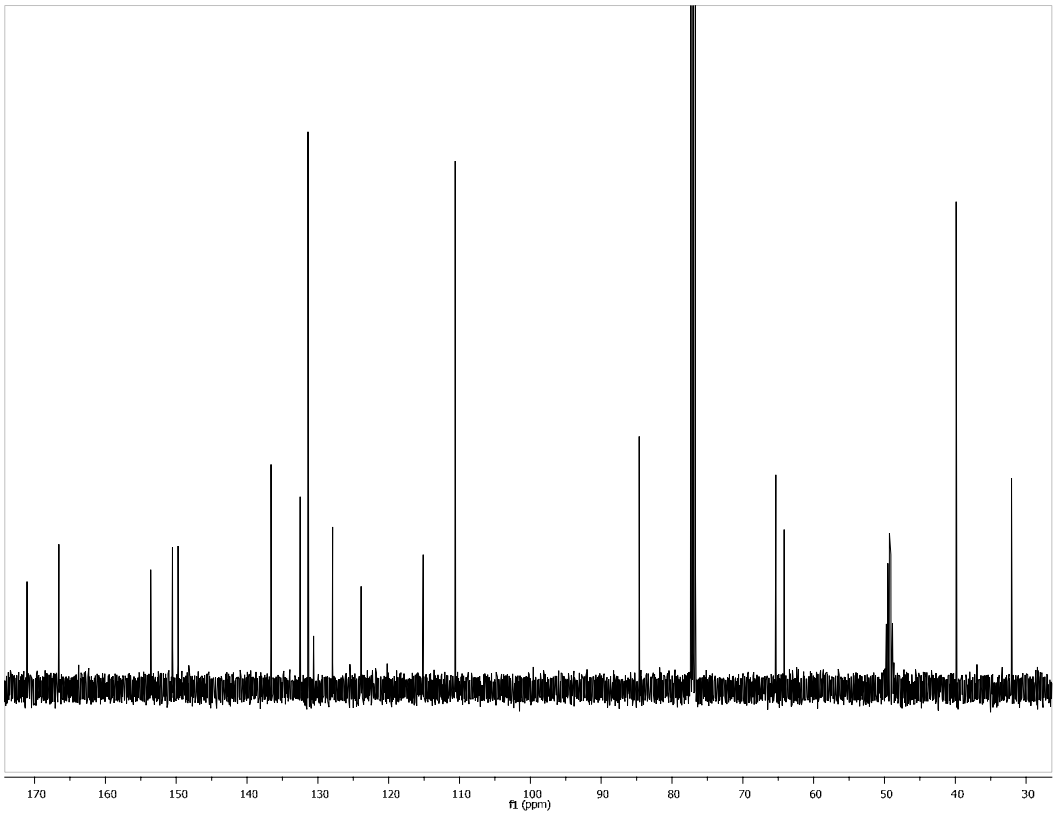
		Calculated			Found		
Compound Number	**Formula**	**C**	**H**	**N**	**C**	**H**	**N**
12k-*E*	$C_{24}H_{21}NO_6$	68.73	5.05	3.34	68.33	5.07	3.42
12k-*Z*	$C_{24}H_{21}NO_6$	68.73	5.05	3.34	68.48	5.09	3.34
12l-*E*	$C_{24}H_{23}NO_6$	68.40	5.50	3.32	68.32	5.59	3.34
12m-*E*	$C_{20}H_{27}NO_5 \bullet 0.2H_2O$	65.81	7.57	3.84	65.79	7.58	3.74
12m-*Z*	$C_{20}H_{27}NO_5 \bullet 0.5H_2O$	64.85	7.62	3.78	64.86	7.53	3.83
12n-*E*	$C_{20}H_{27}NO_5$	66.46	7.53	3.88	66.33	7.59	3.93
12n-*Z*	$C_{20}H_{27}NO_5$	66.46	7.53	3.88	66.20	7.59	3.66
12o-*E*	$C_{20}H_{27}NO_5 \bullet 0.7H_2O$	64.11	7.30	3.70	64.00	7.33	3.81
12o-*Z*	$C_{20}H_{27}NO_5 \bullet 0.2H_2O$	65.81	7.57	3.83	65.51	7.49	3.77
12p-*E*	$C_{24}H_{29}NO_5 \bullet 0.2H_2O$	69.44	7.14	3.37	69.21	7.23	3.37
12p-*Z*	$C_{24}H_{29}NO_5 \bullet 0.4H_2O$	68.85	7.17	3.35	68.88	7.06	3.33
12q-*E*	$C_{24}H_{29}NO_5 \bullet 0.8H_2O$	67.68	7.24	3.29	67.84	6.98	3.21
12q-*Z*	$C_{24}H_{29}NO_5 \bullet 0.3H_2O$	69.14	7.16	3.36	69.01	6.89	3.29
12r-*E*	$C_{24}H_{31}NO_5 \bullet 0.6H_2O$	67.93	7.65	3.30	67.74	7.54	3.11
12s-*E*	$C_{23}H_{33}NO_5$	68.46	8.24	3.47	68.40	8.54	3.31
12t-*E*	$C_{27}H_{37}NO_5 \bullet 0.1H_2O$	70.90	8.20	3.06	70.71	8.18	3.04





^{1}H and ^{13}C spectra of **12a-*E***





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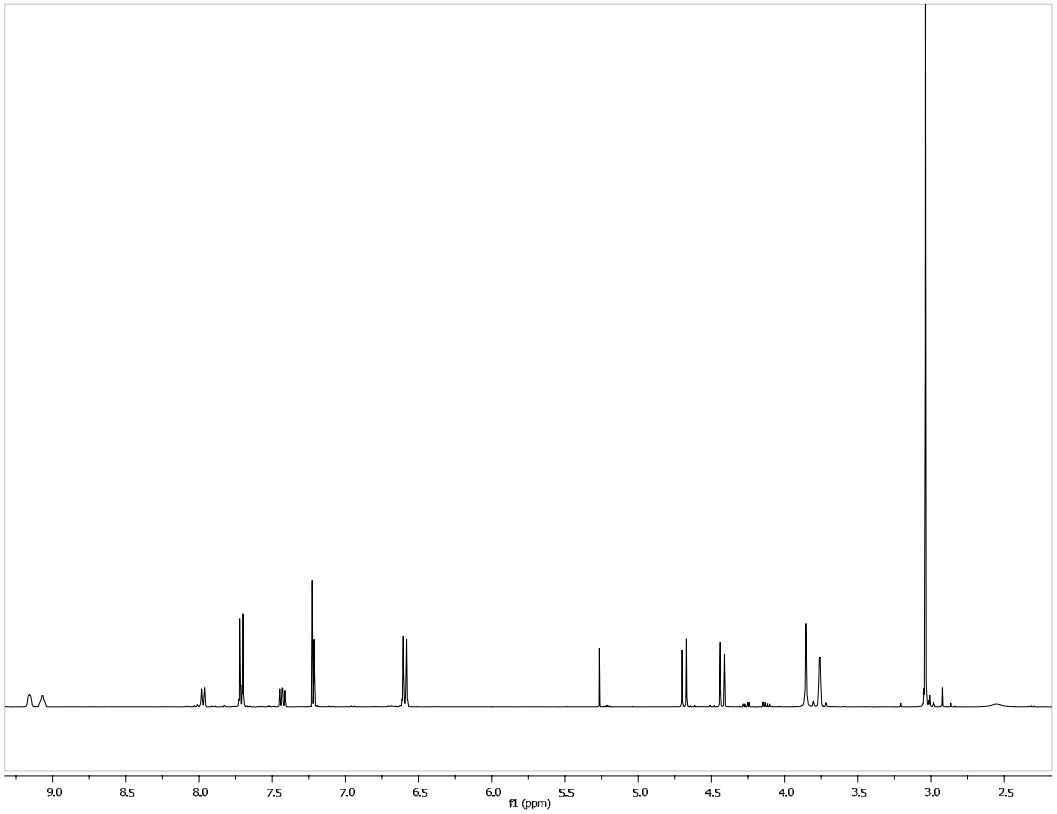
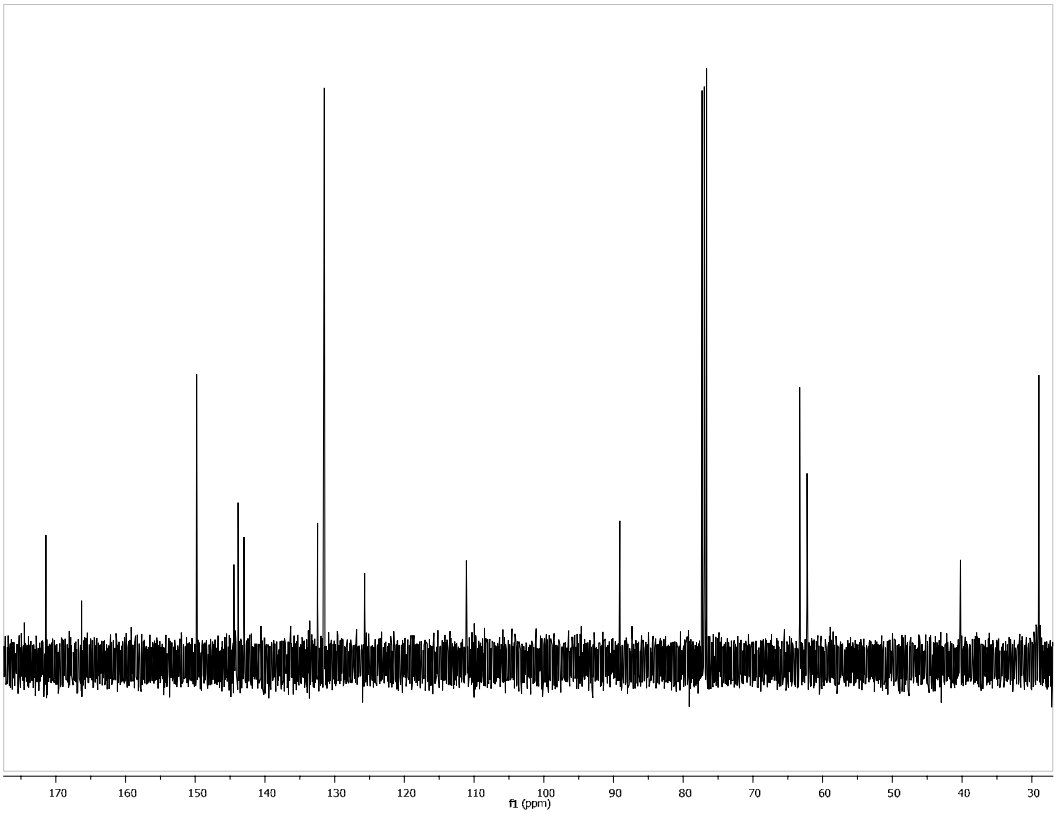
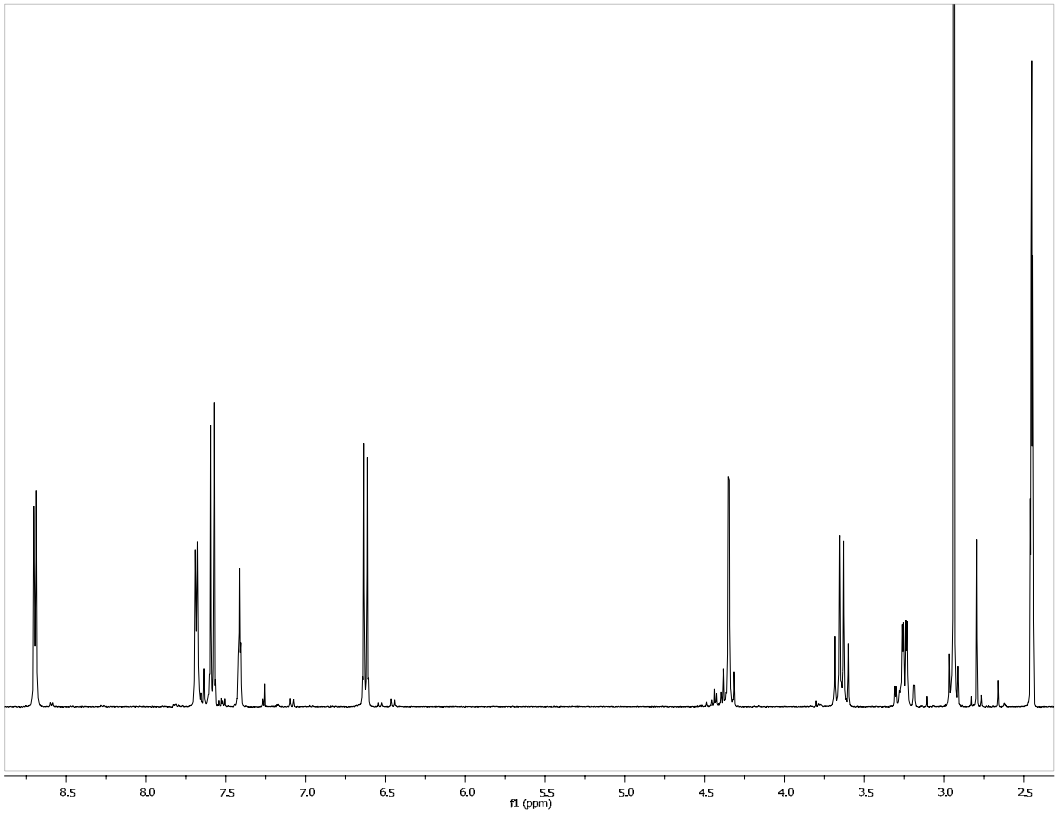
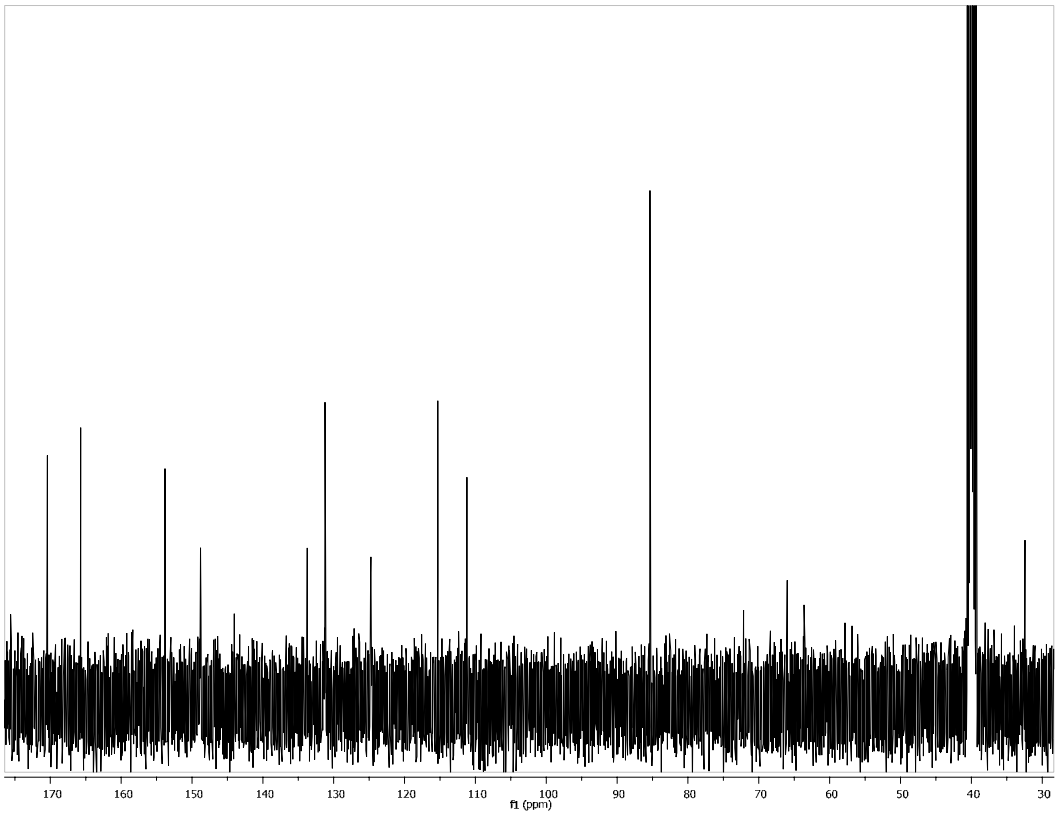




^{1}H and ^{13}C spectra of **12b-*Z***





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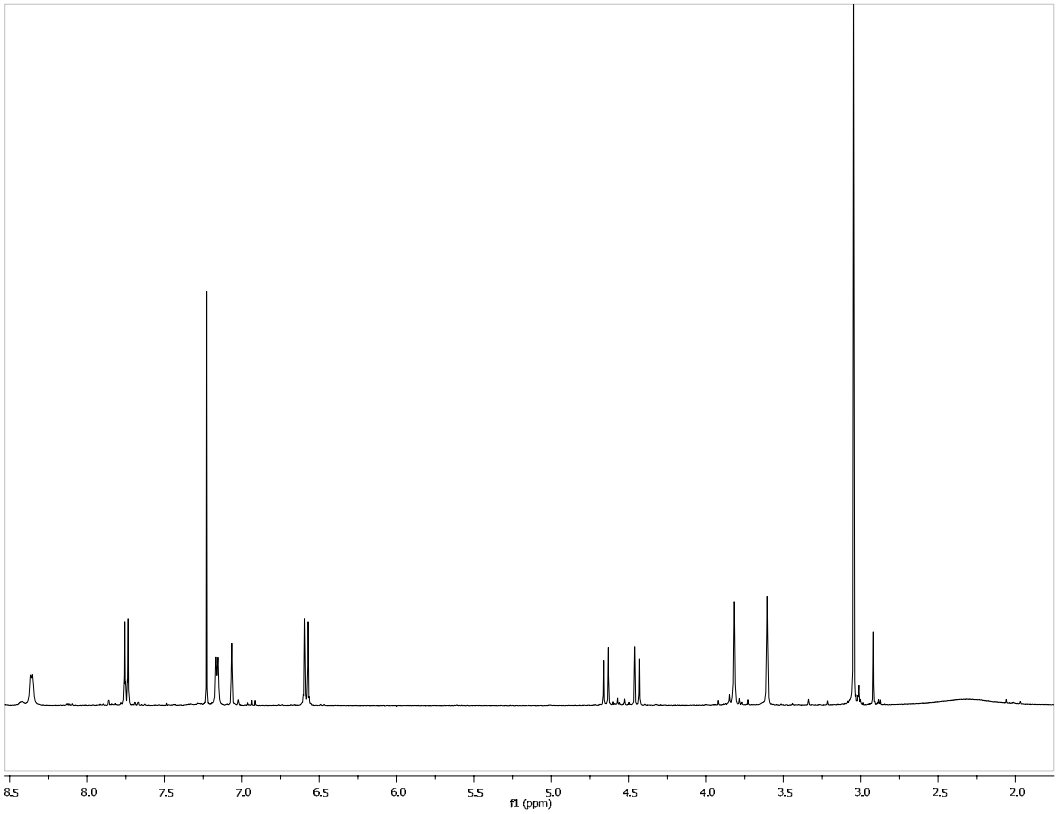
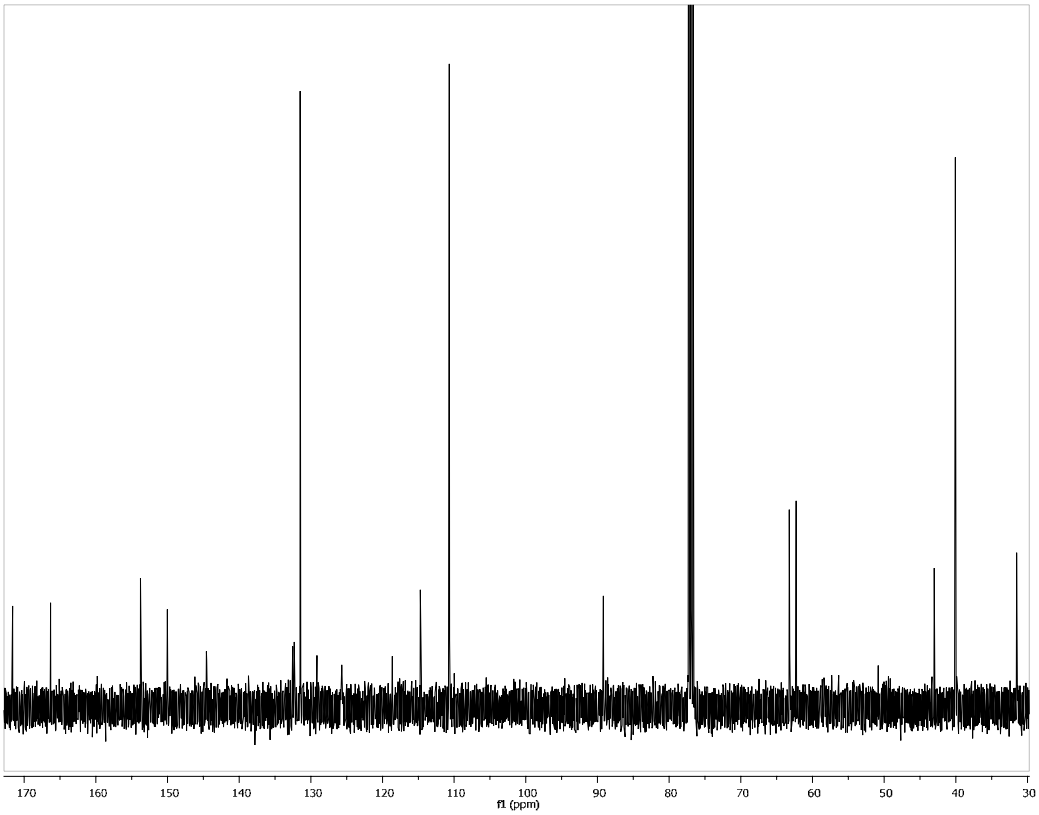
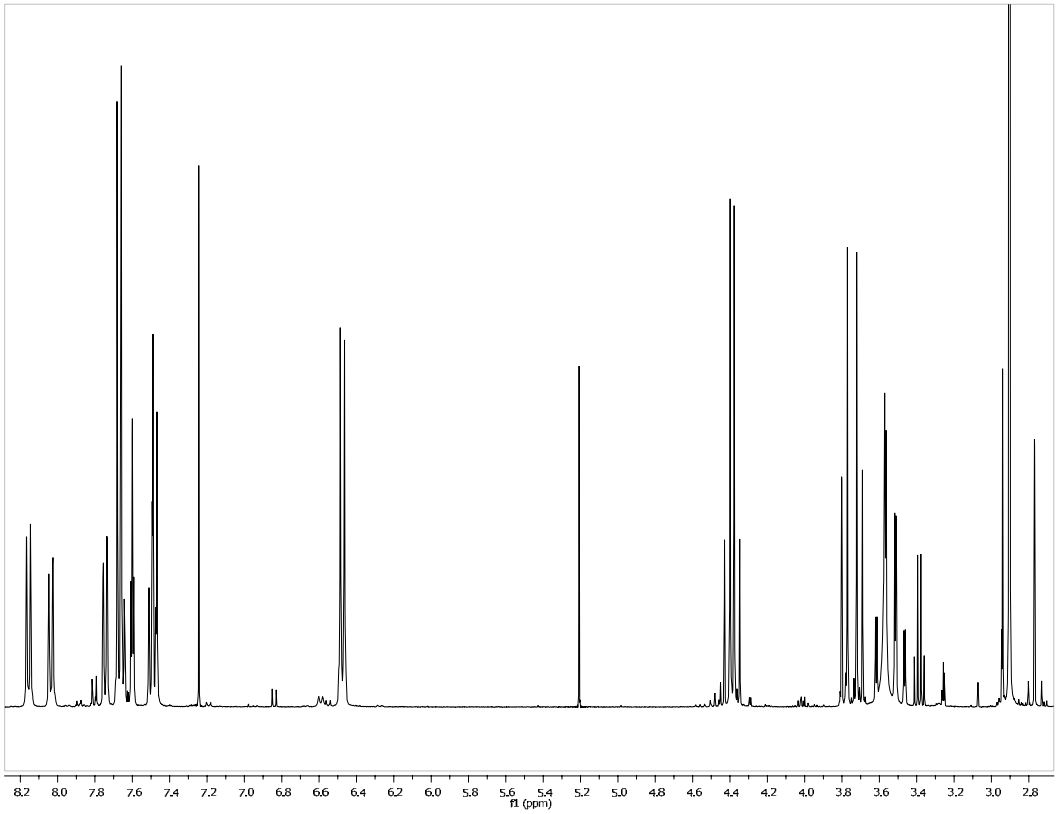
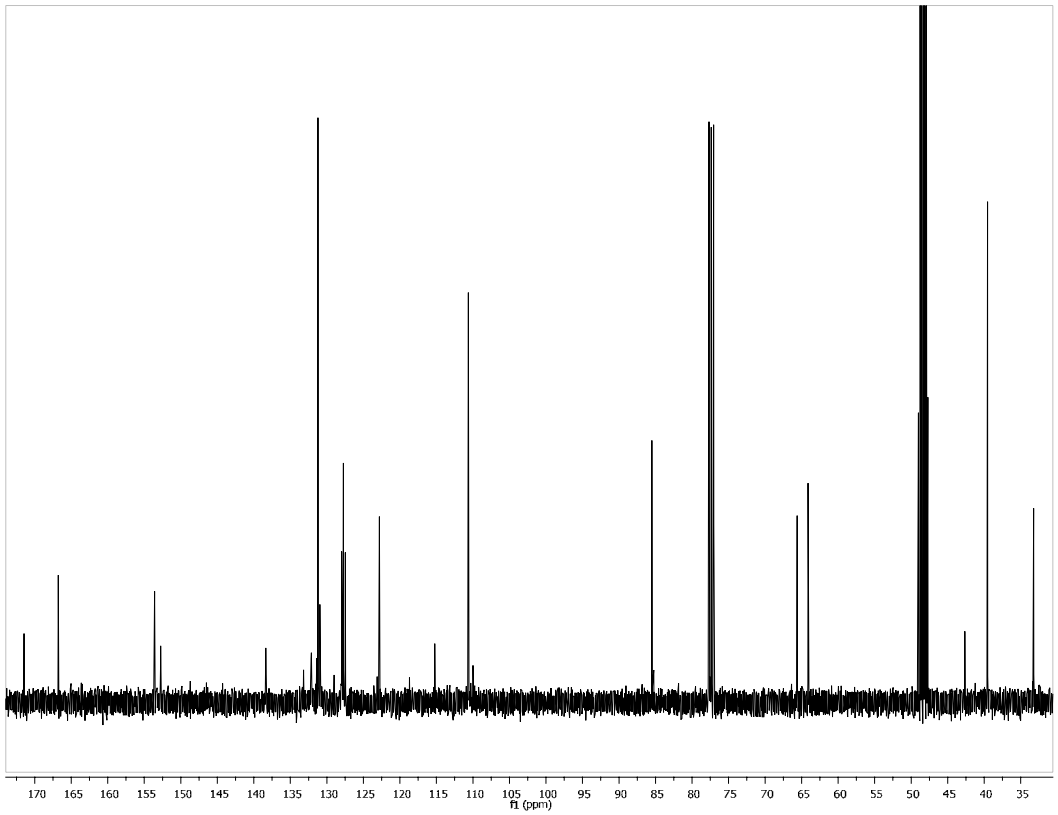




^{1}H and ^{13}C spectra of **12c-*Z***





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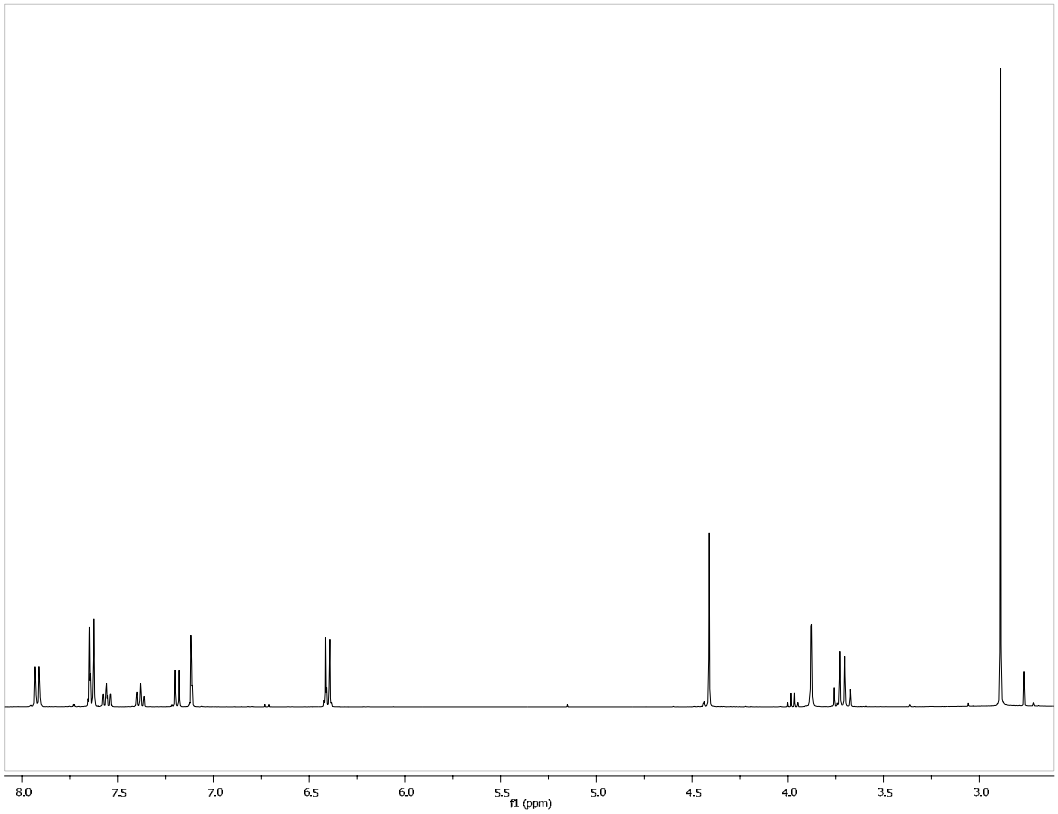
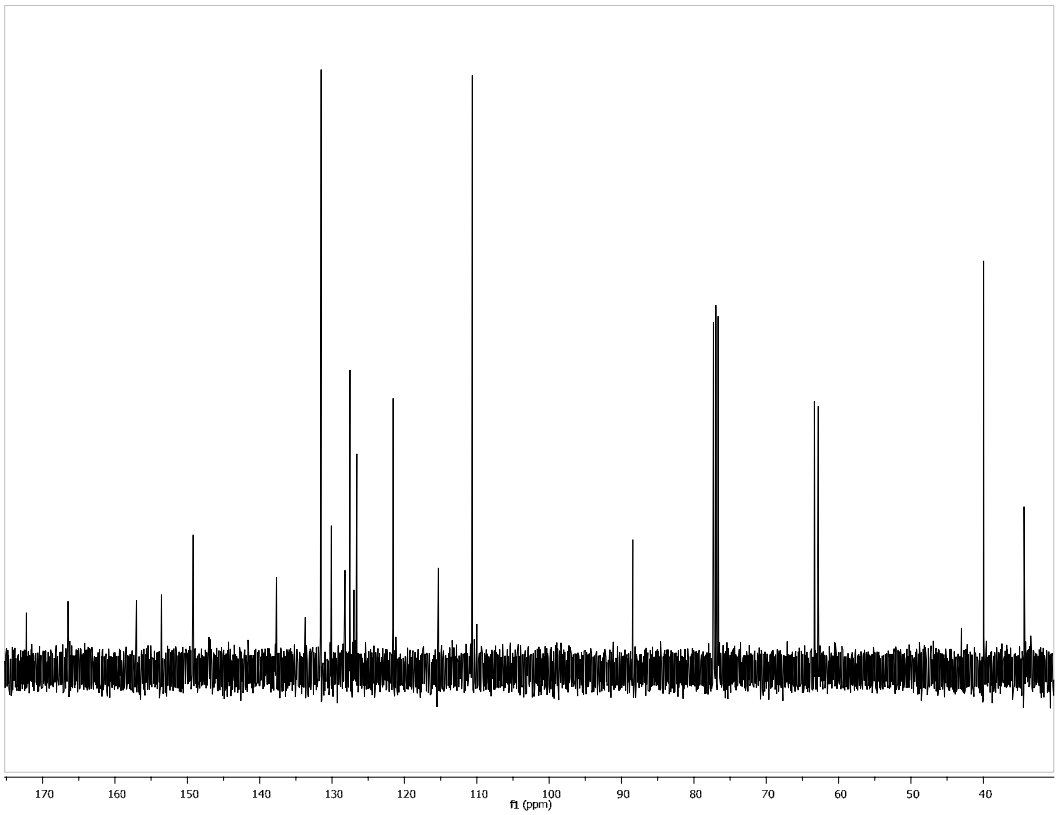
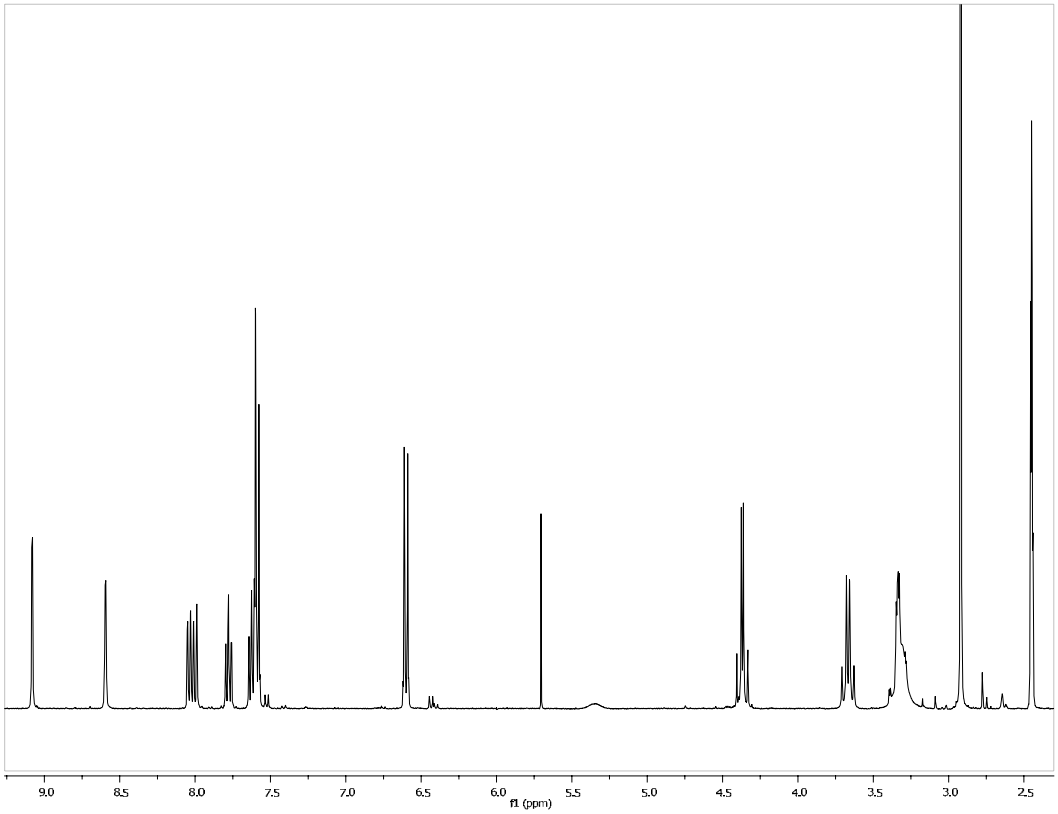
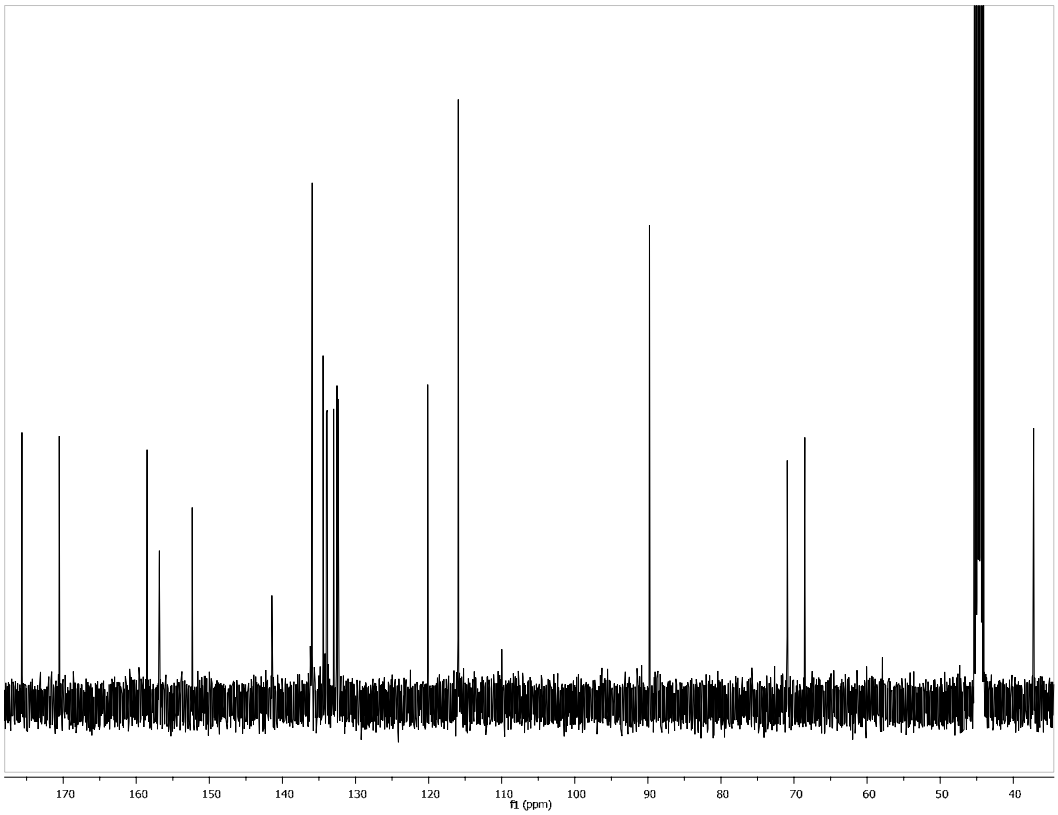


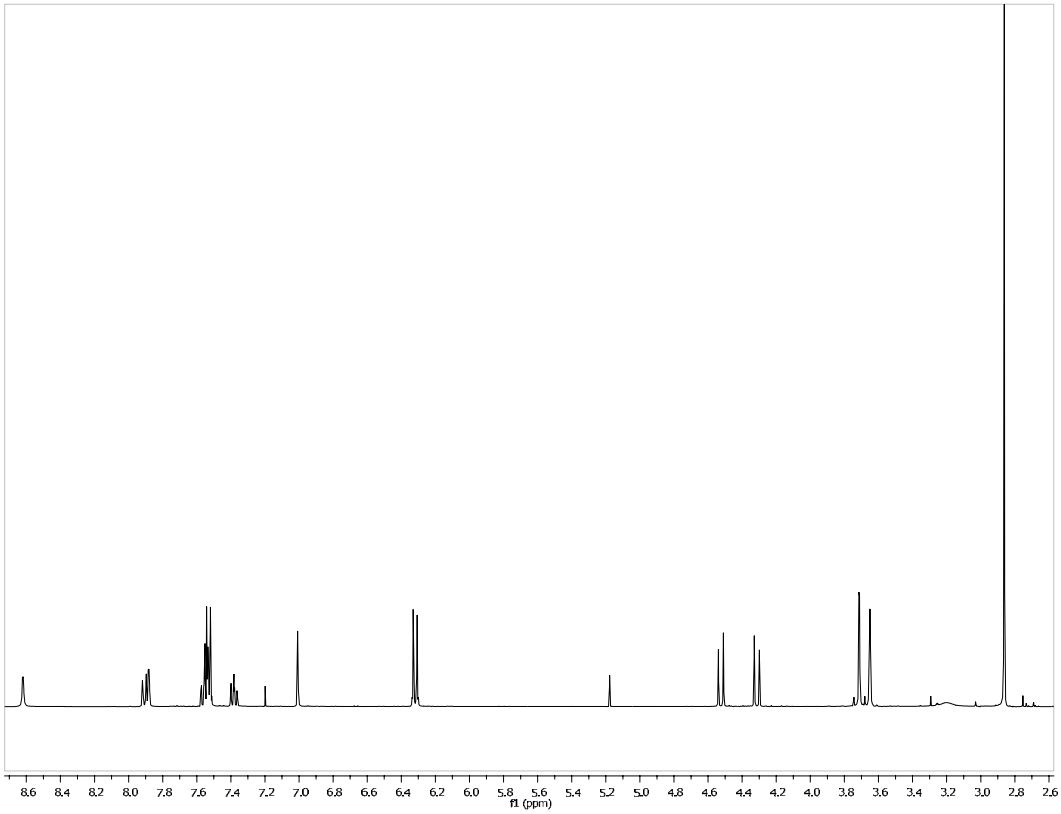


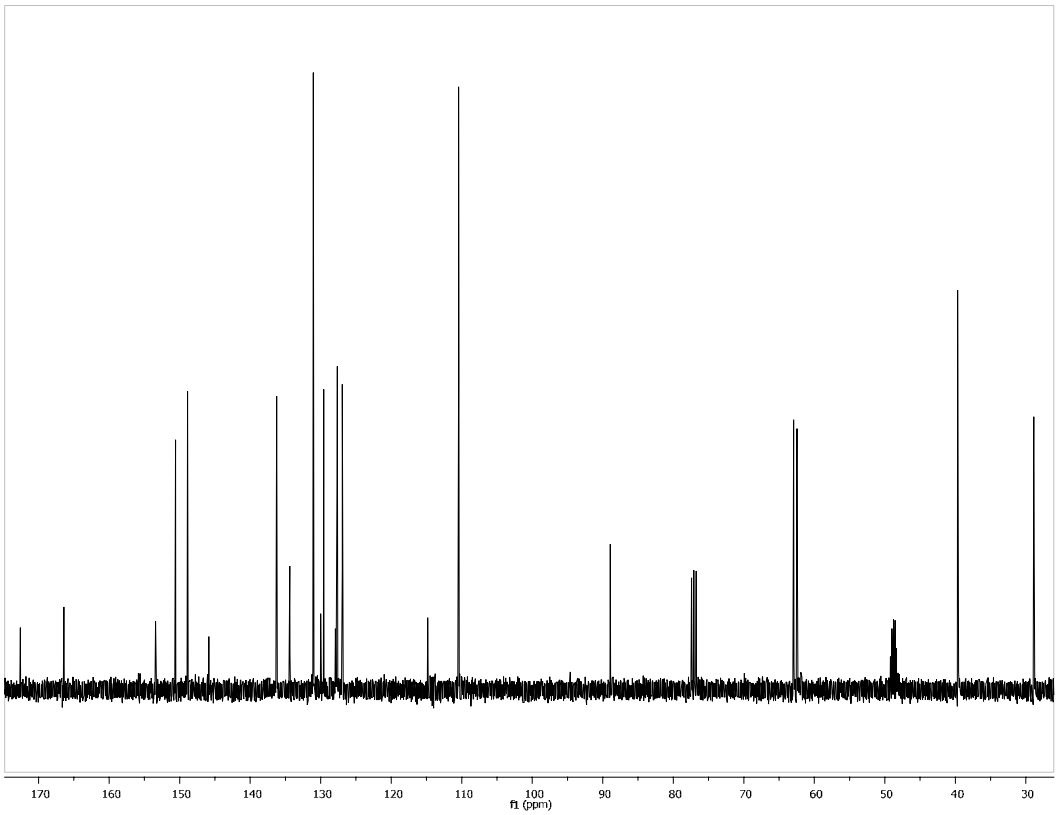
^{1}H and ^{13}C spectra **of 12d-*Z***



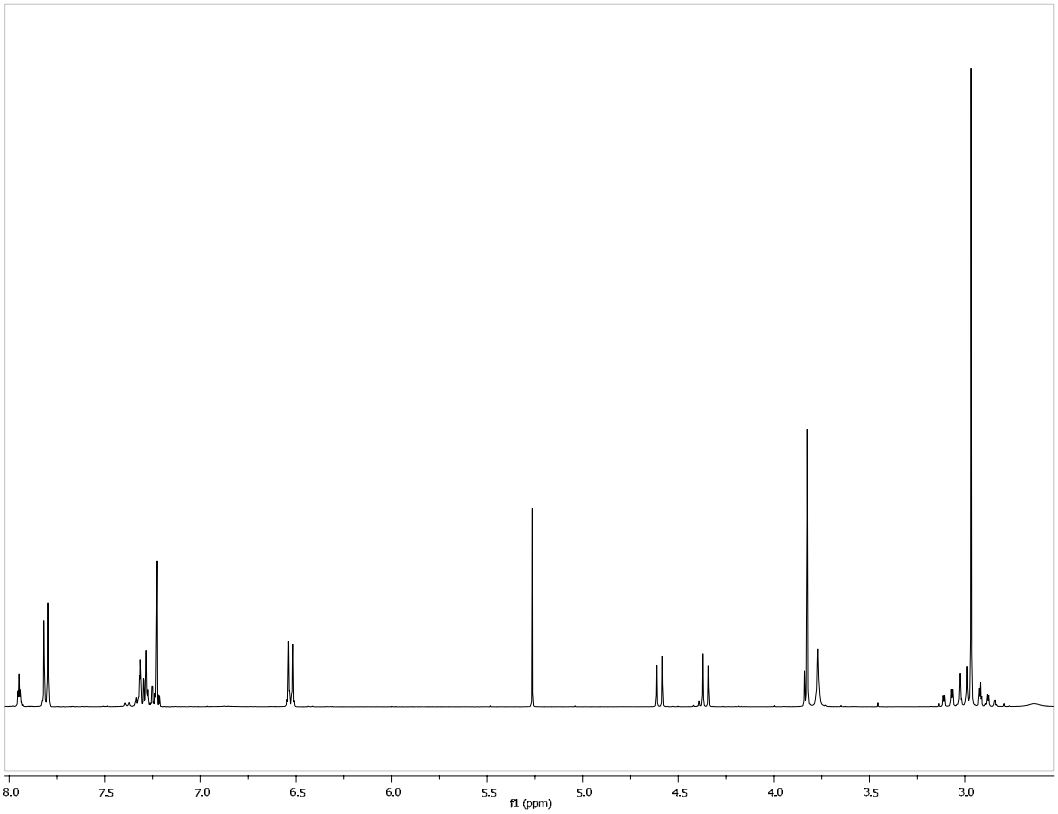


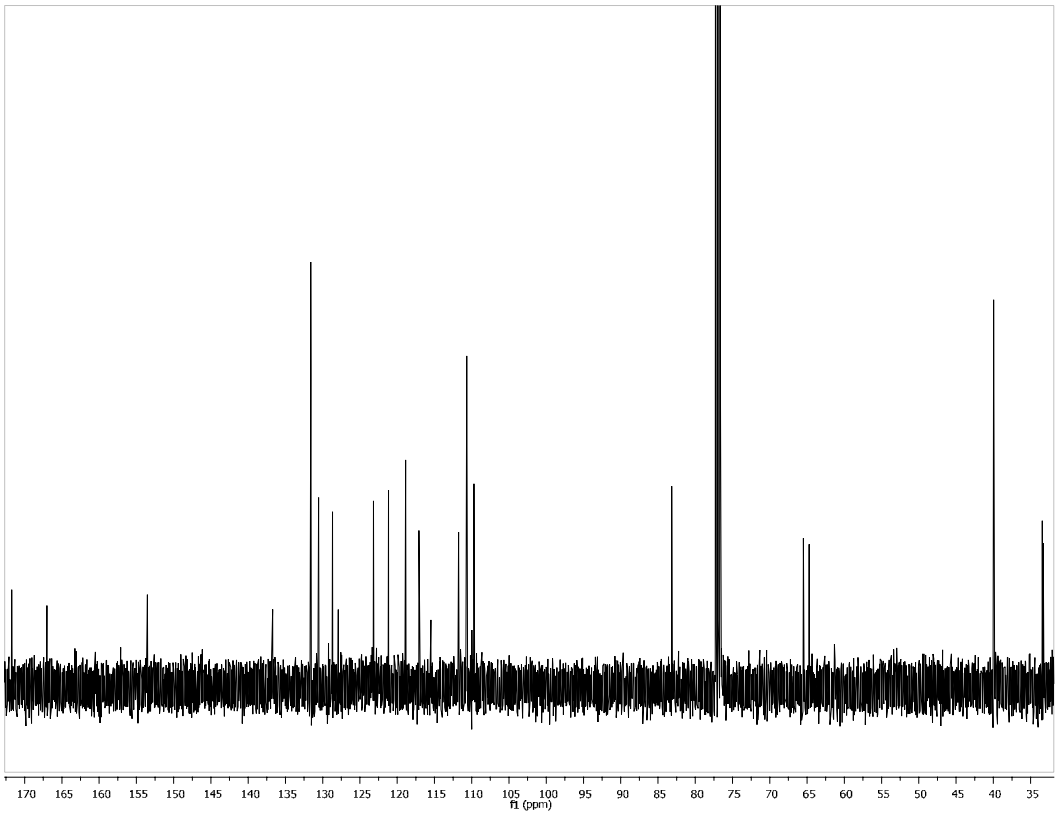
^{1}H and ^{13}C spectra of **12e-*E***



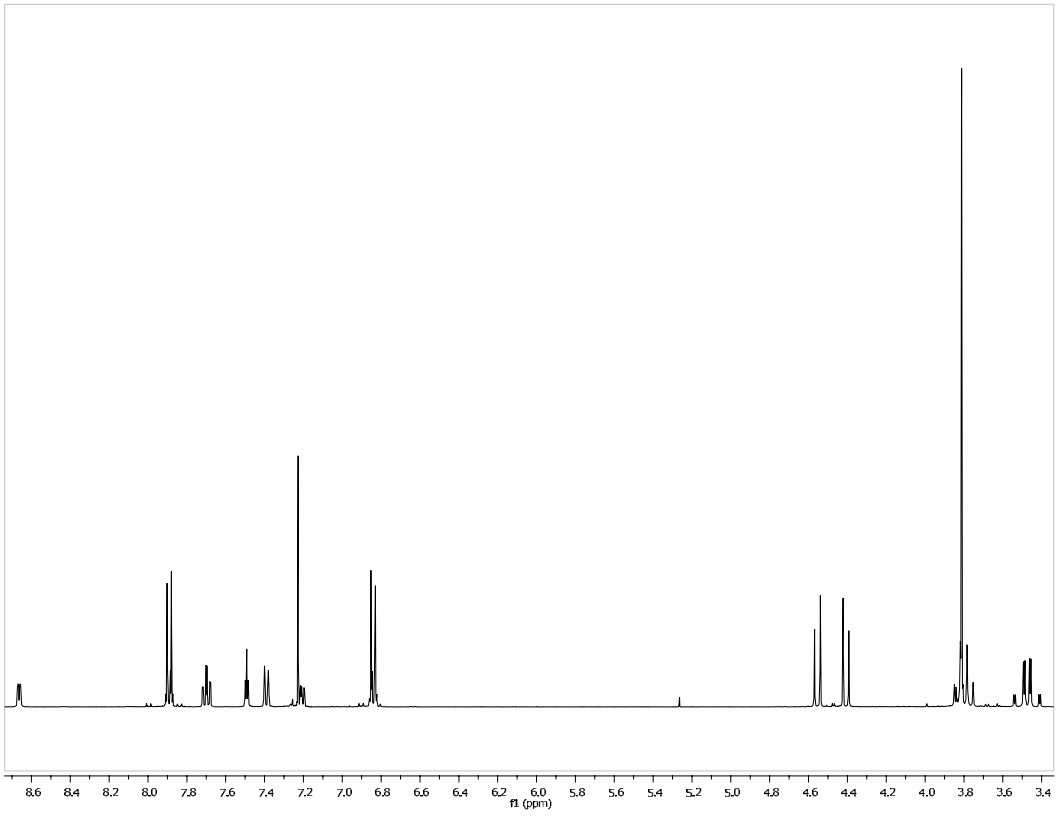


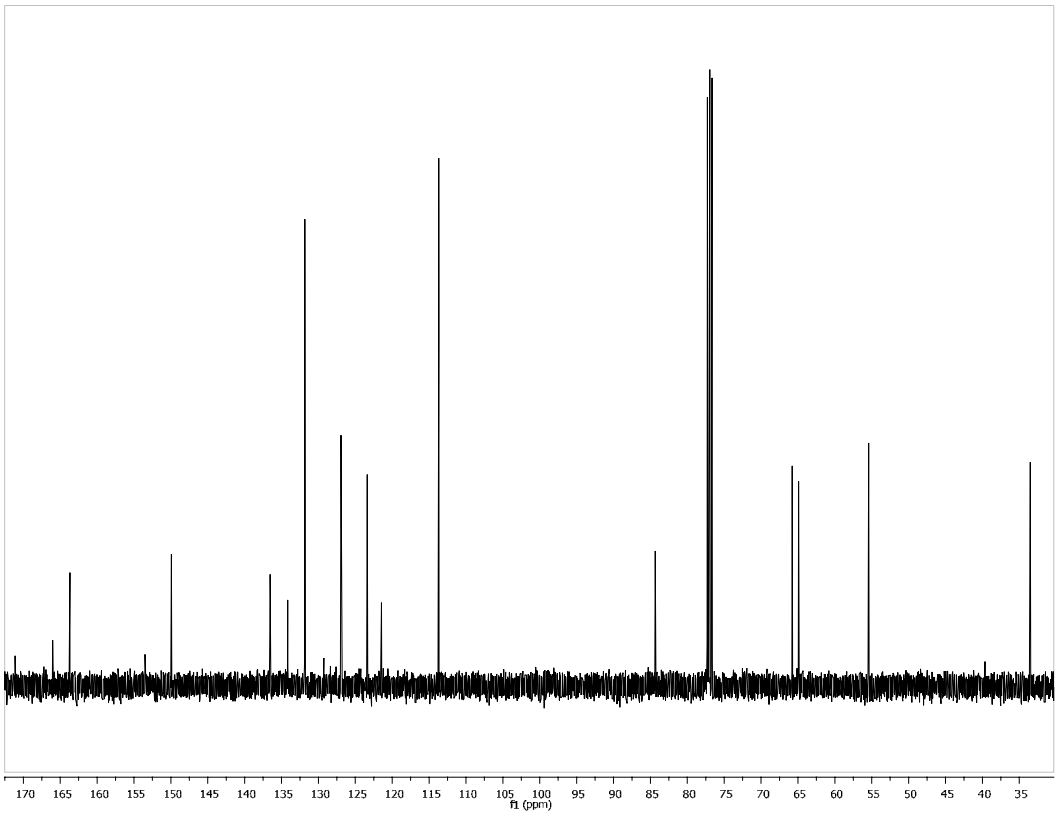
^{1}H and ^{13}C spectra of **12e-*Z***



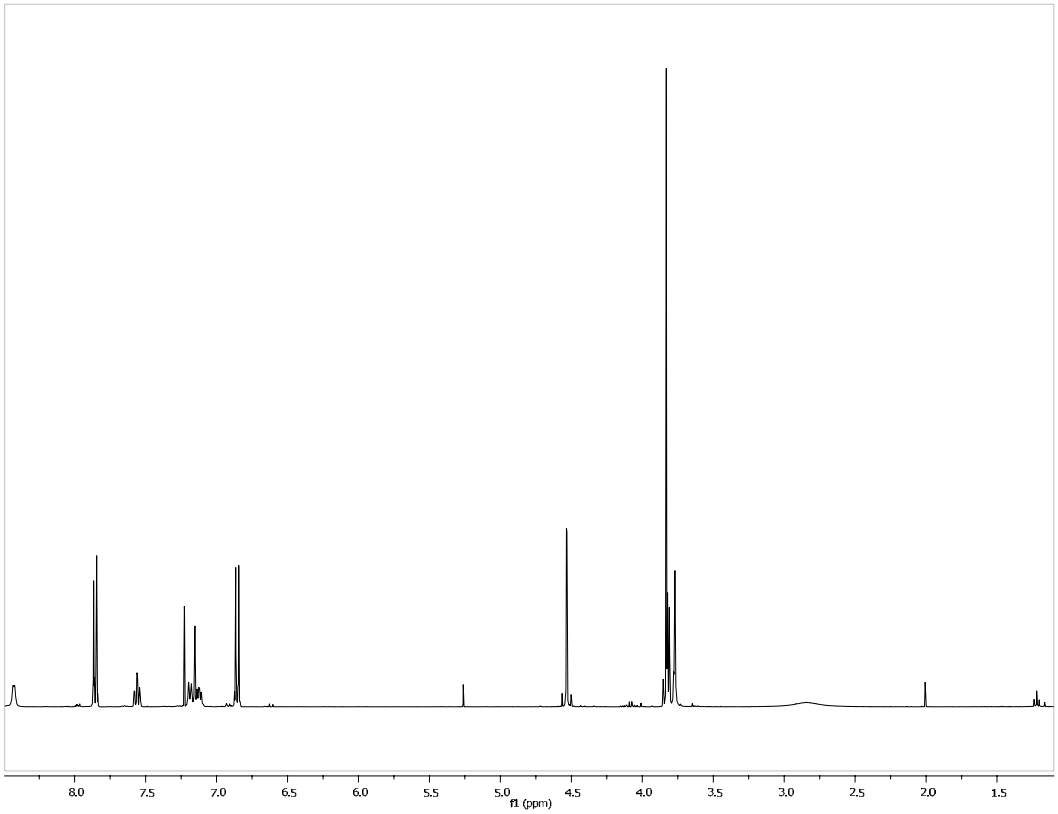


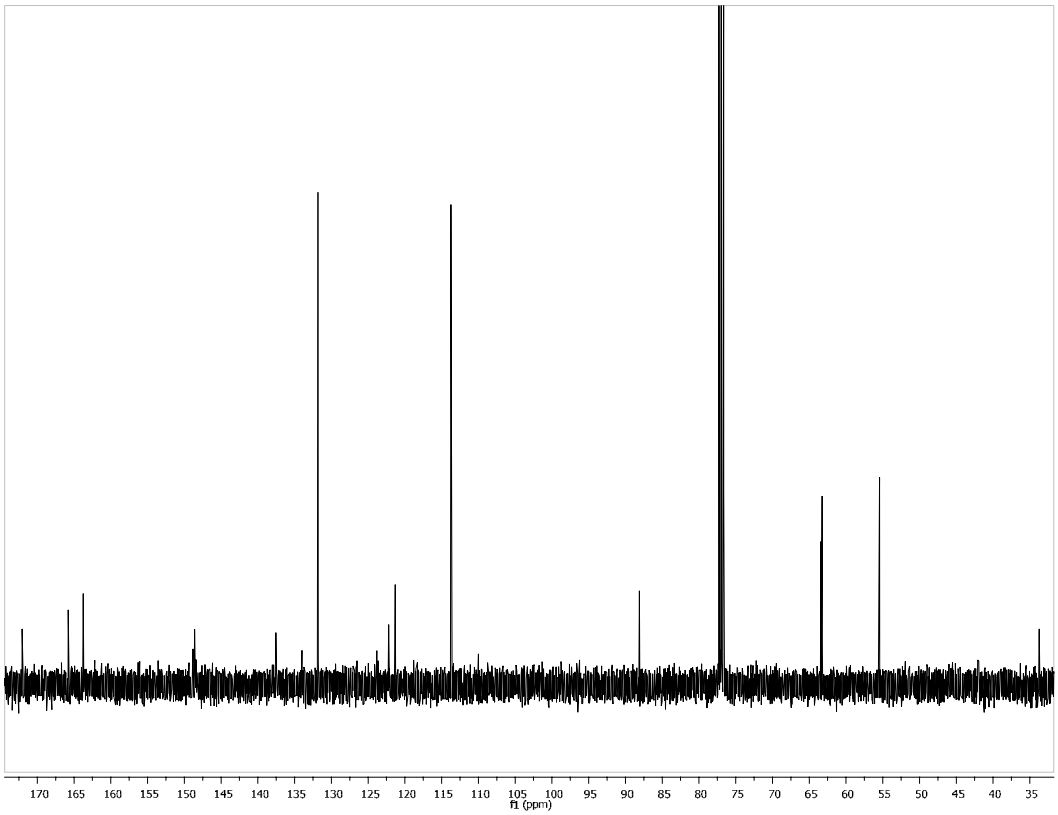
^{1}H and ^{13}C spectra of **12f-*E***



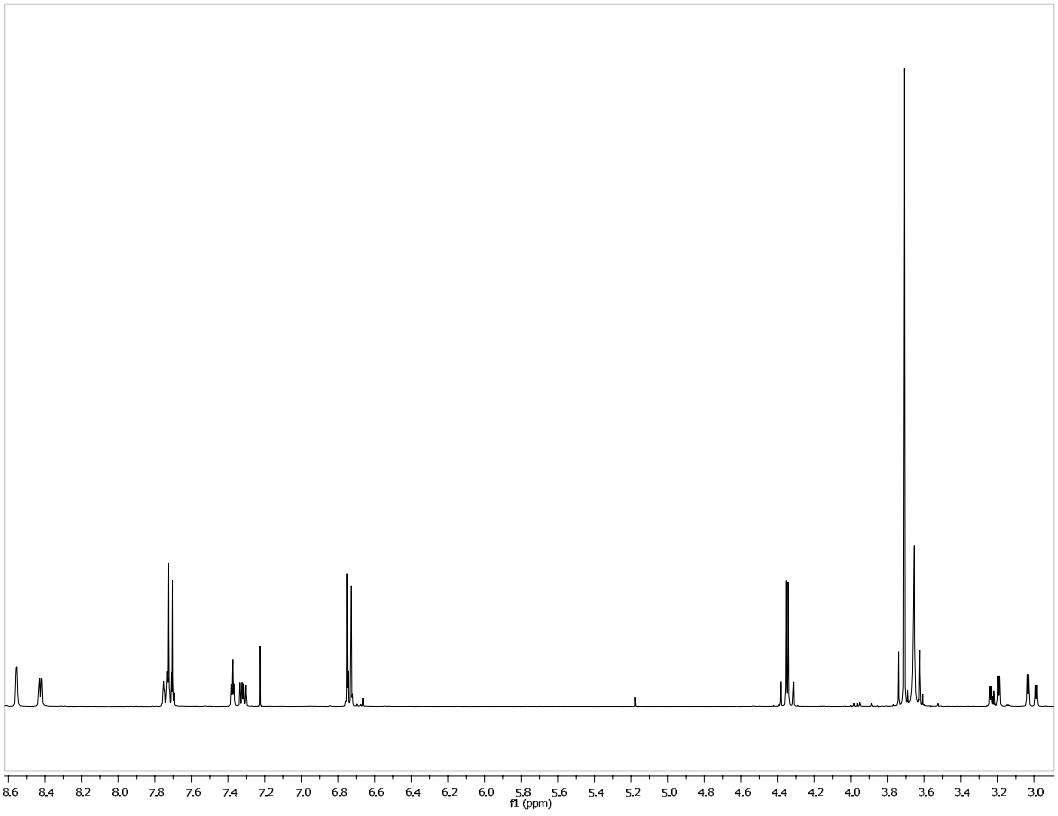


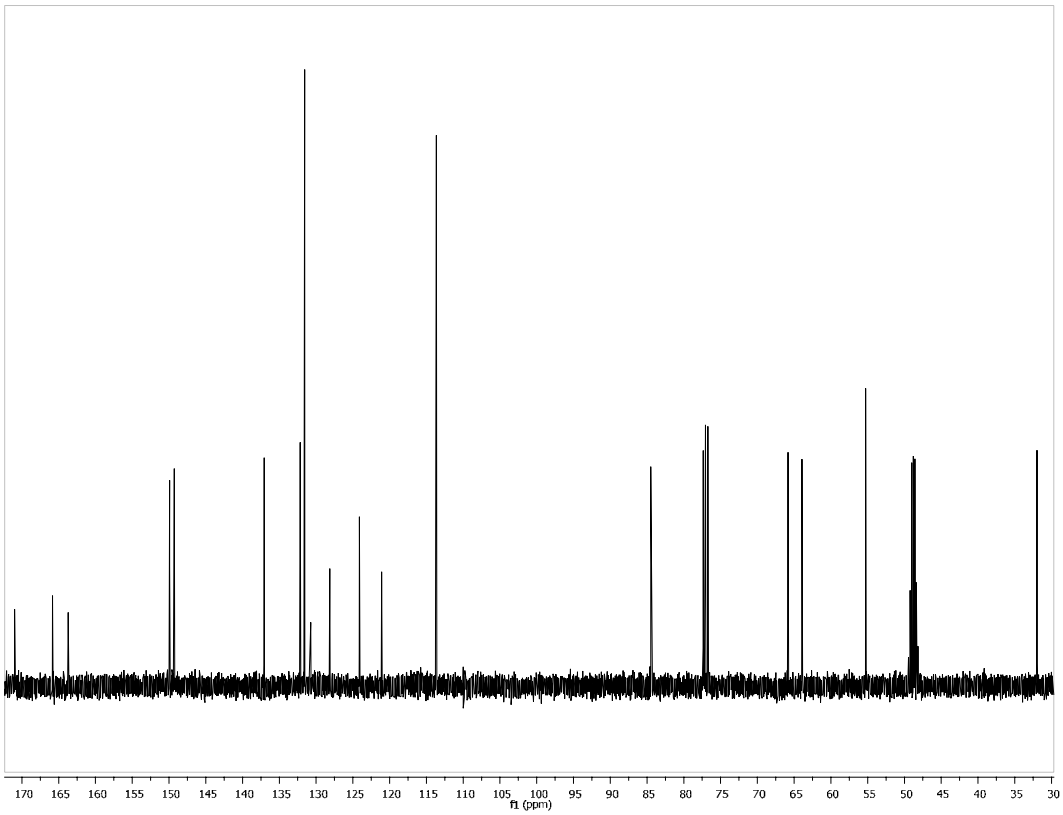
^{1}H and ^{13}C spectra of **12g-*E***



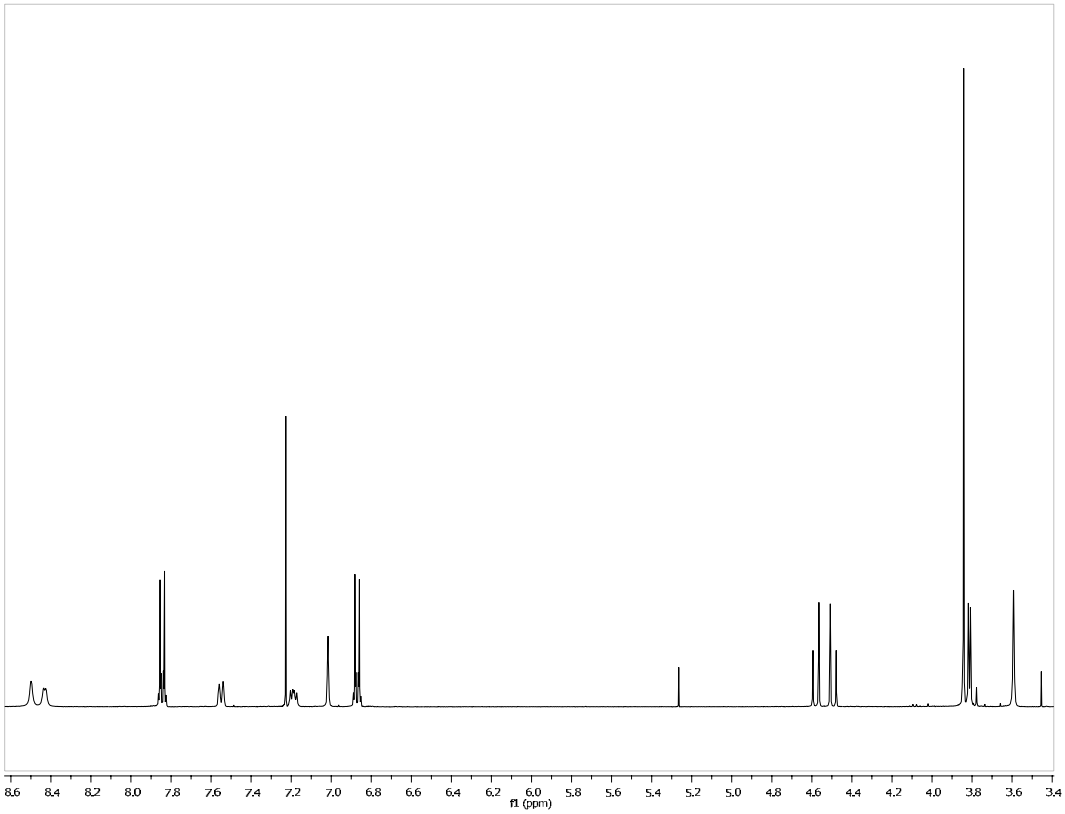


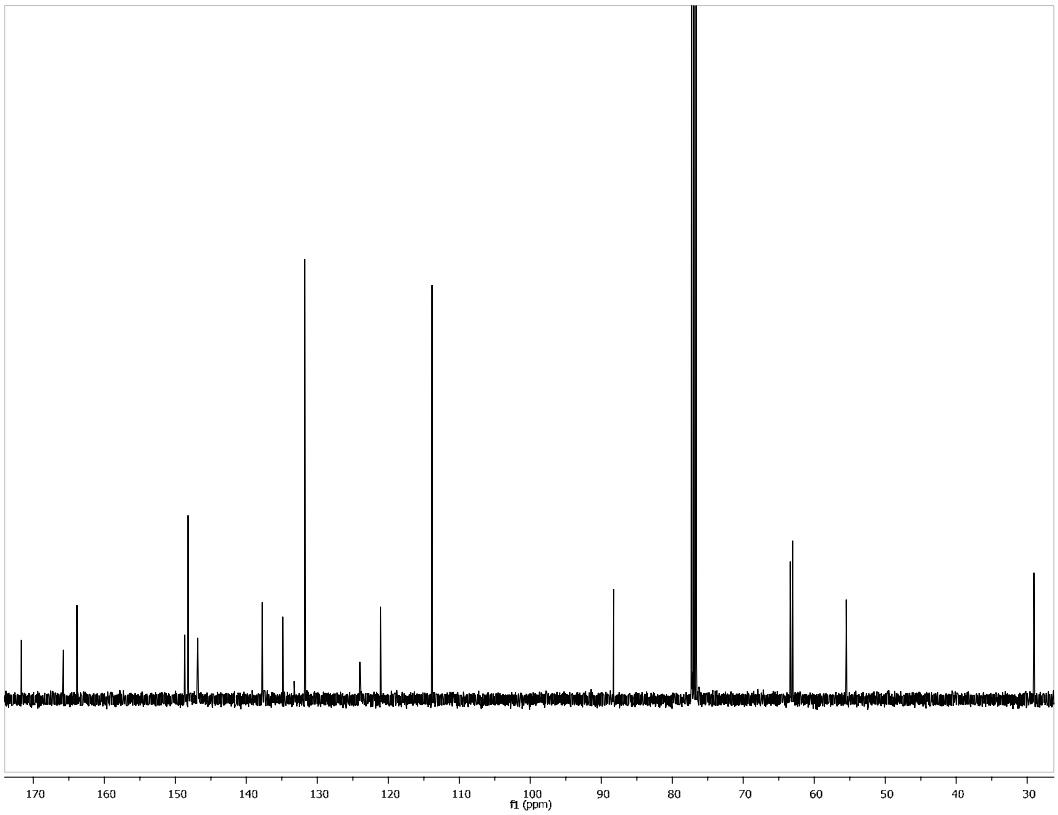
^{1}H and ^{13}C spectra of **12g-*Z***



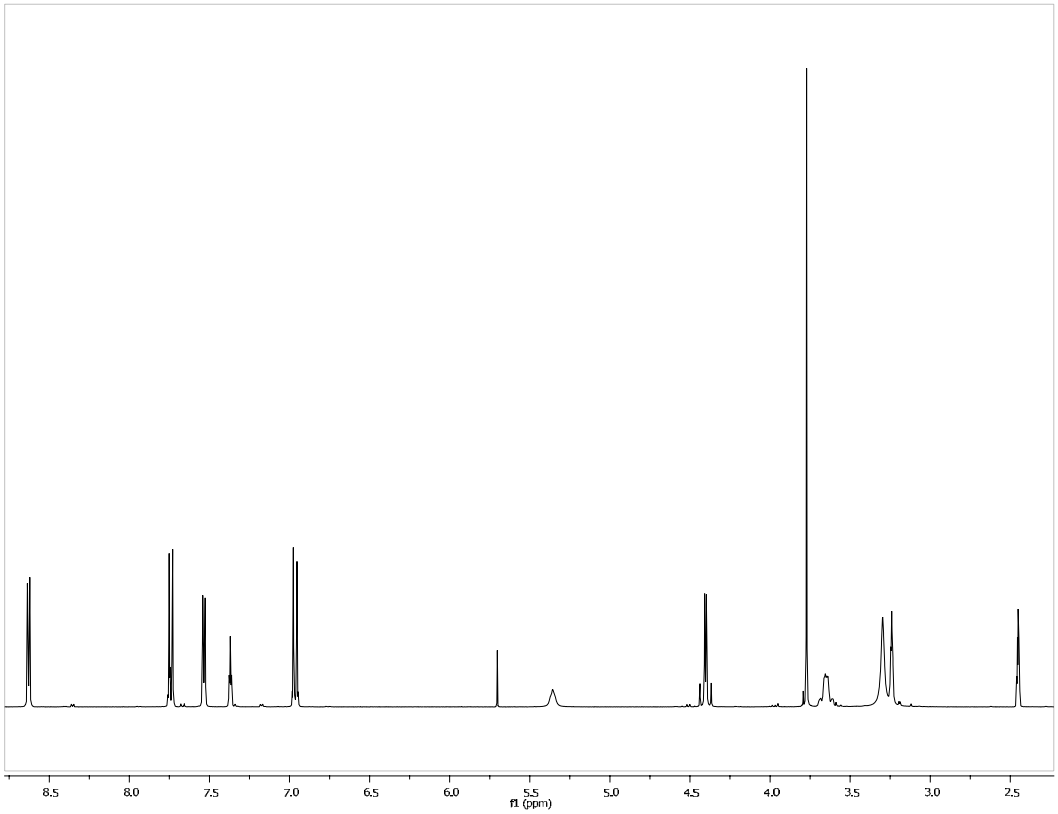


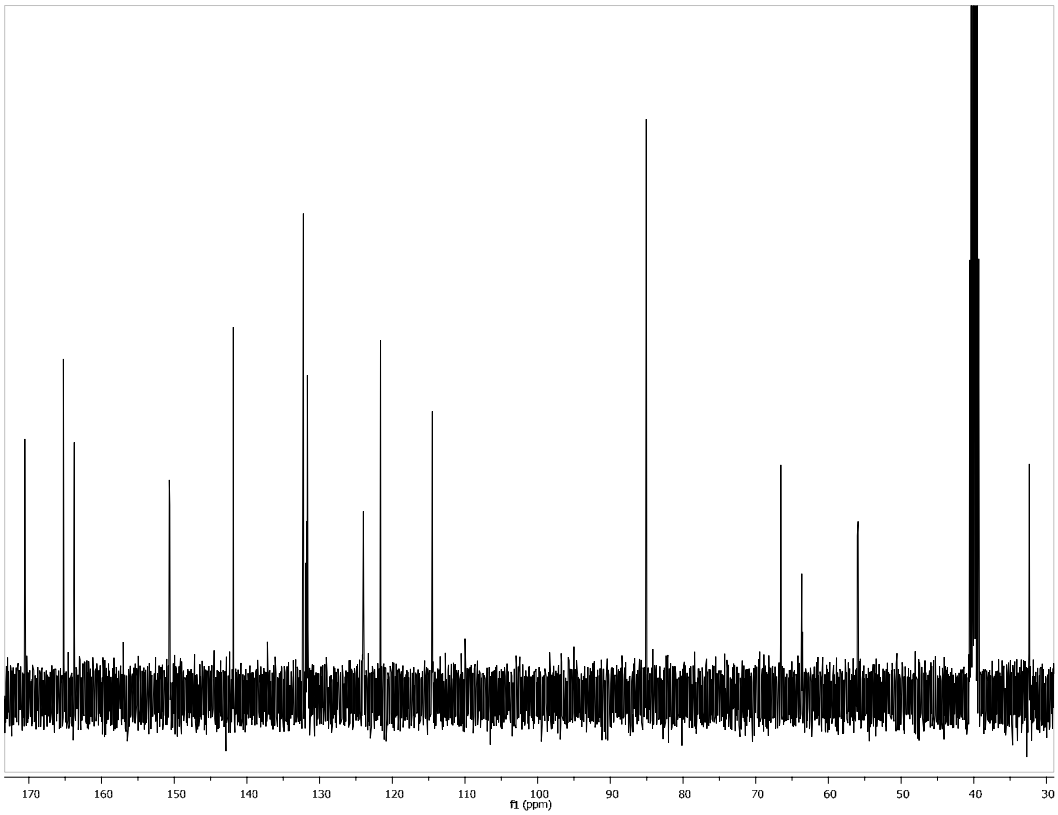
^{1}H and ^{13}C spectra of **12h-*E***



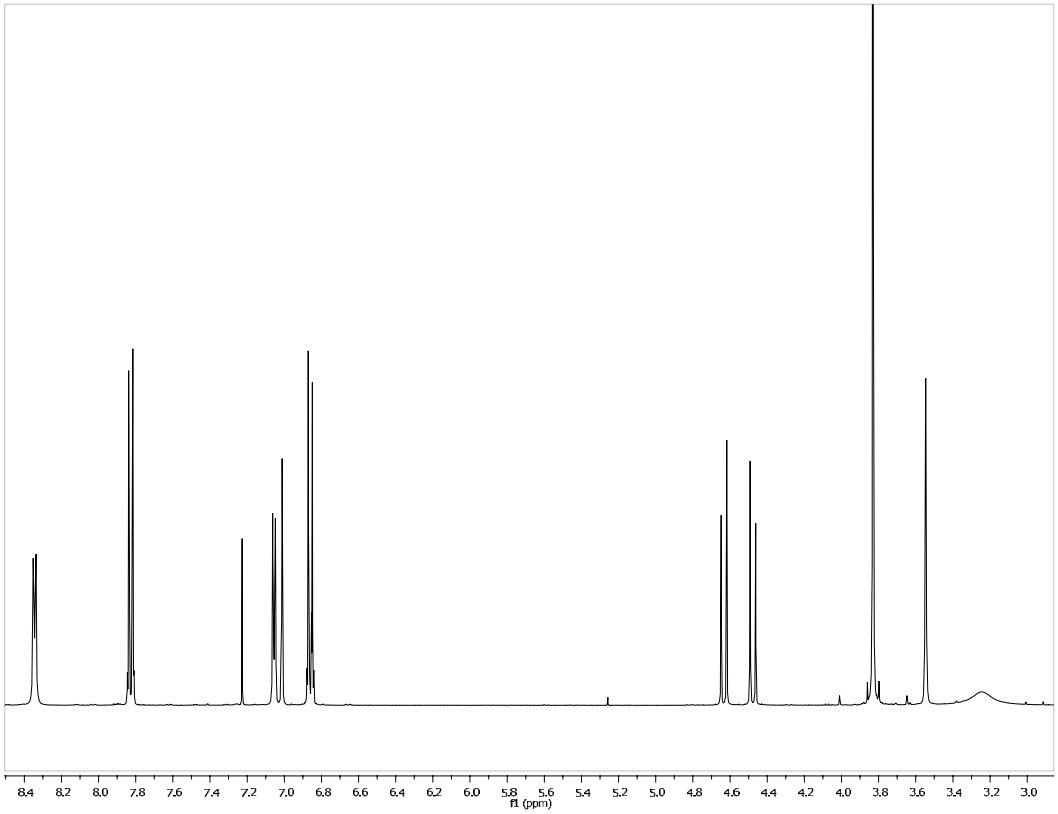


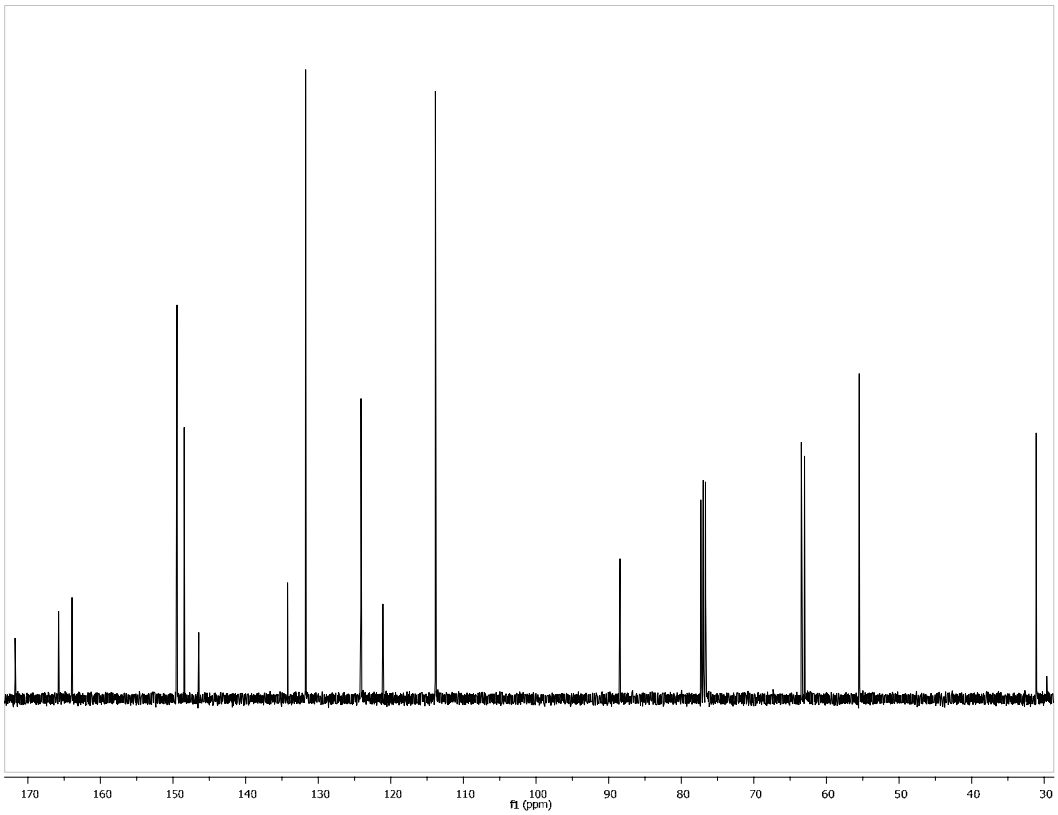
^{1}H and ^{13}C spectra of **12h-*Z***



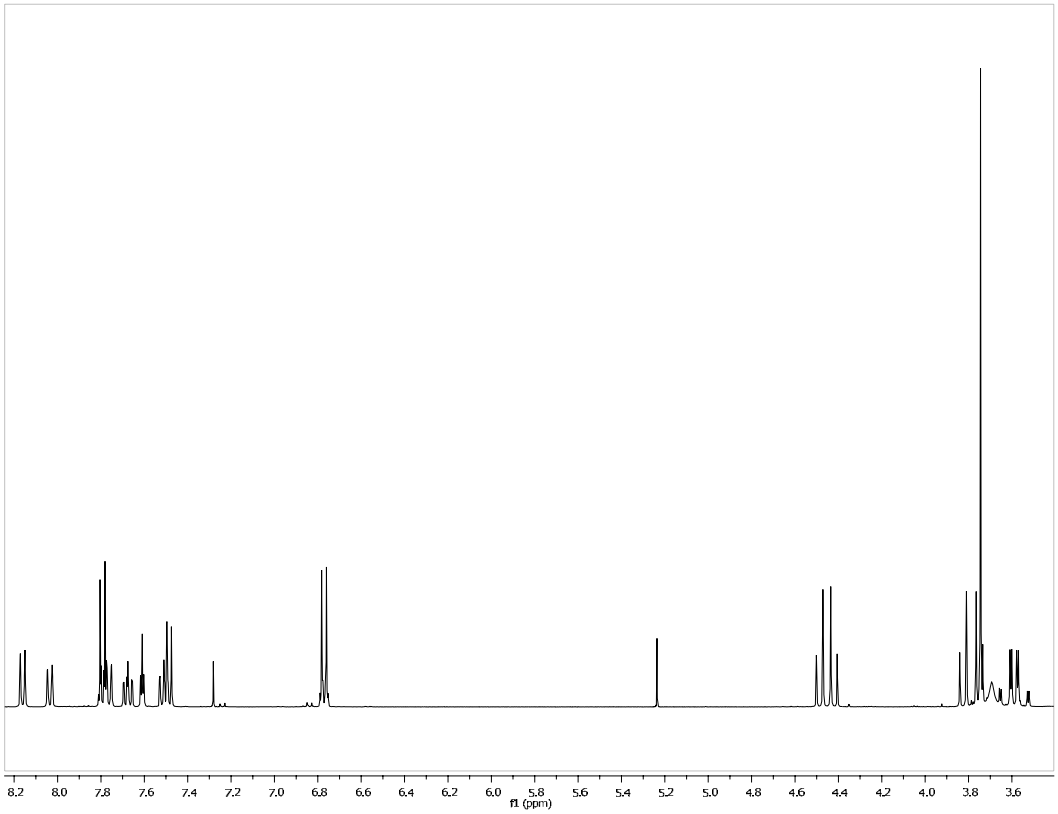


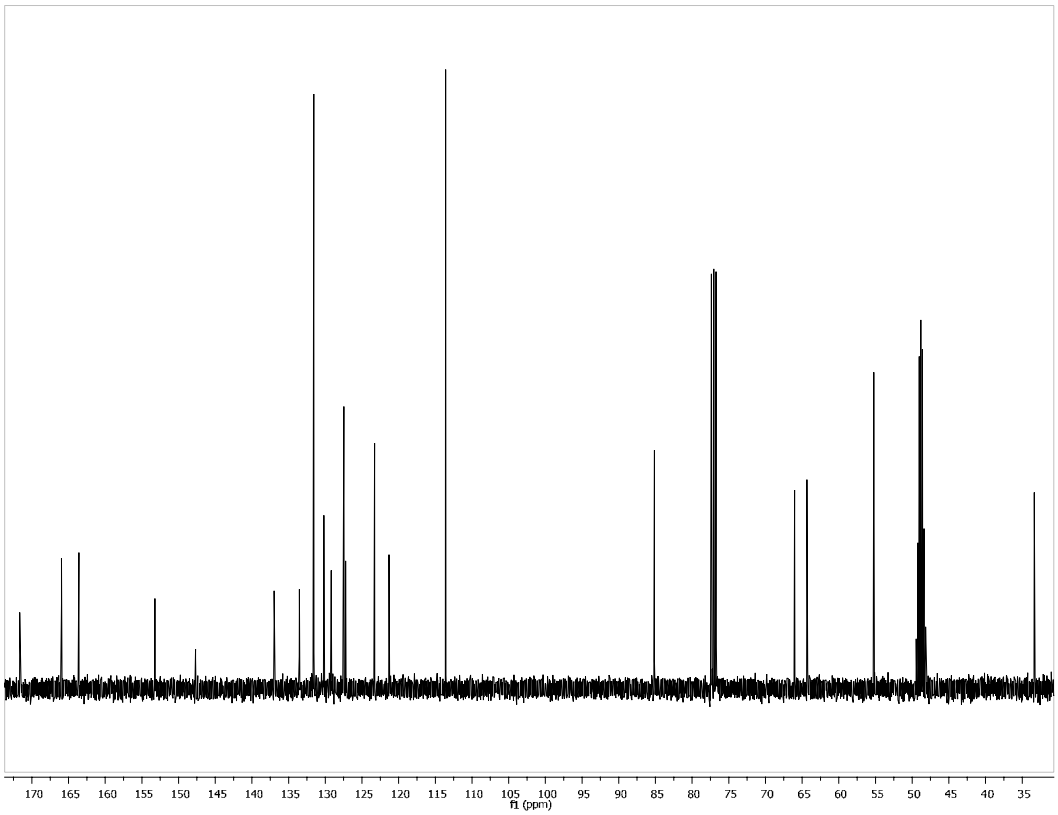
^{1}H and ^{13}C spectra of **12i-*E***



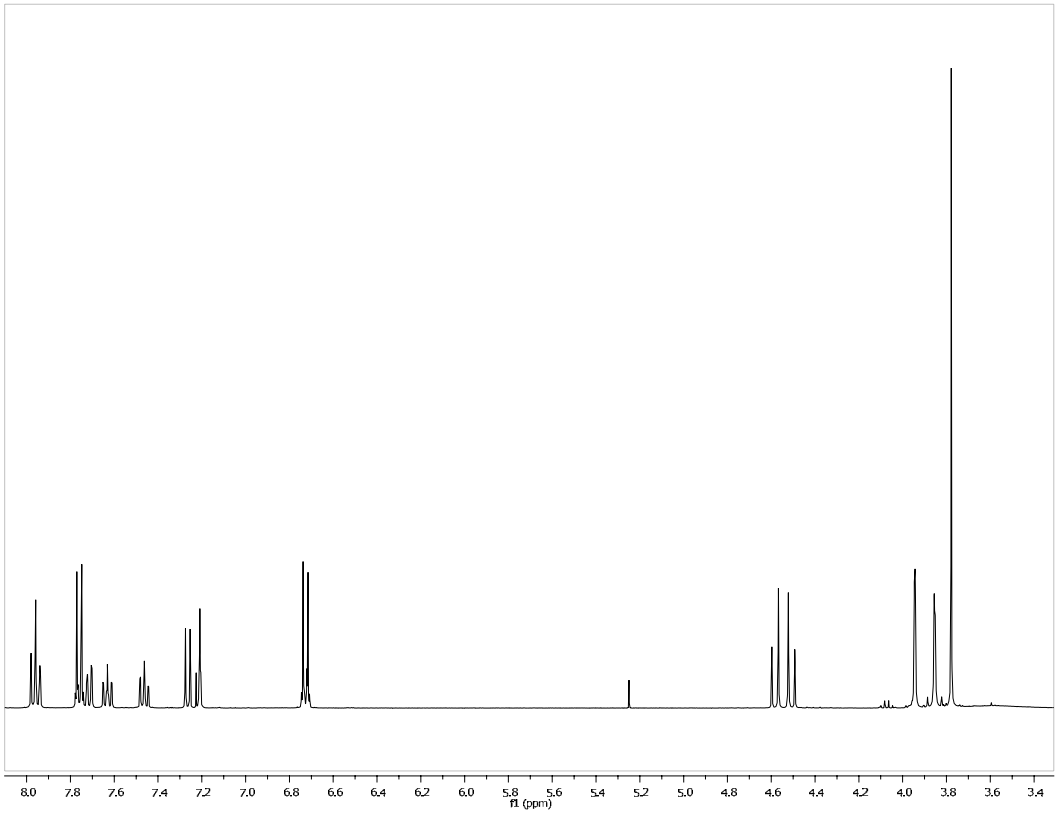


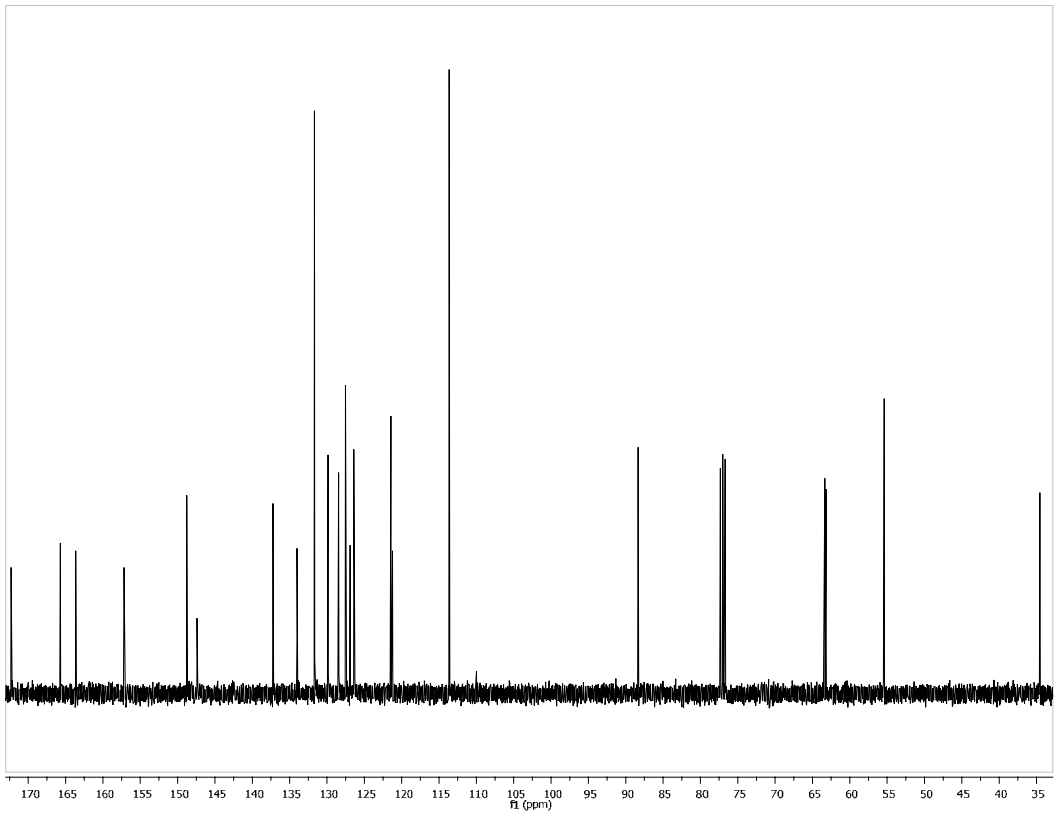
^{1}H and ^{13}C spectra of **12i-*Z***



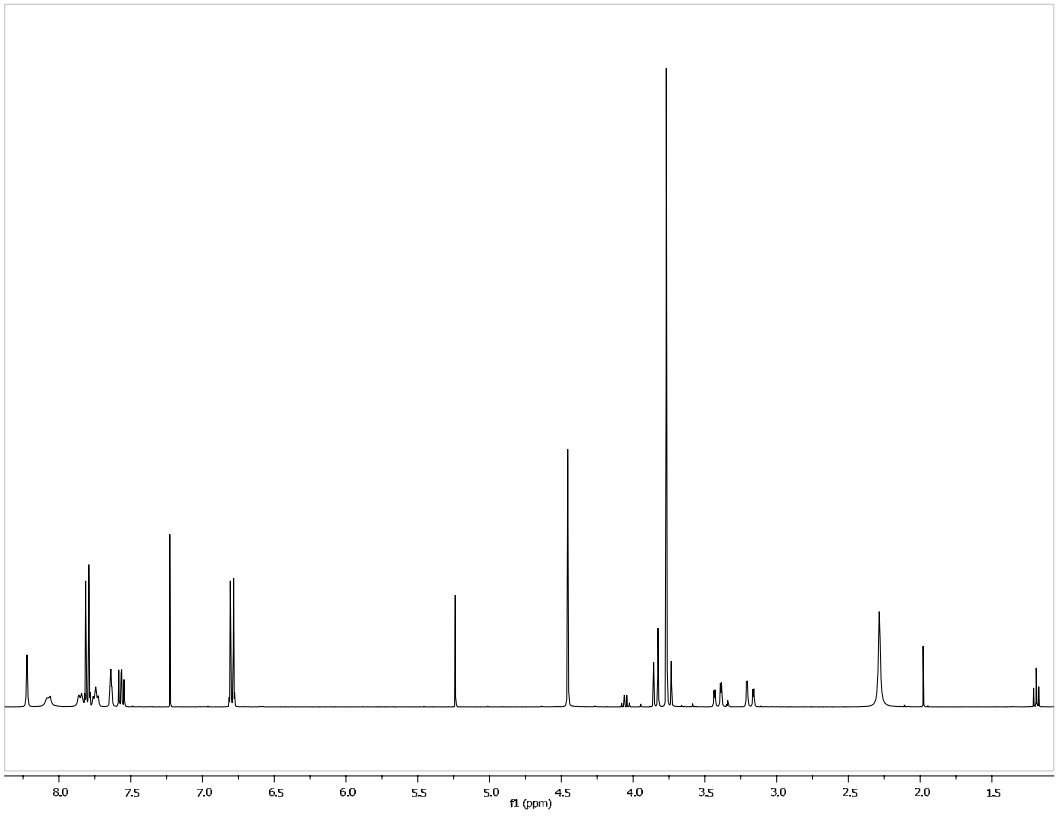


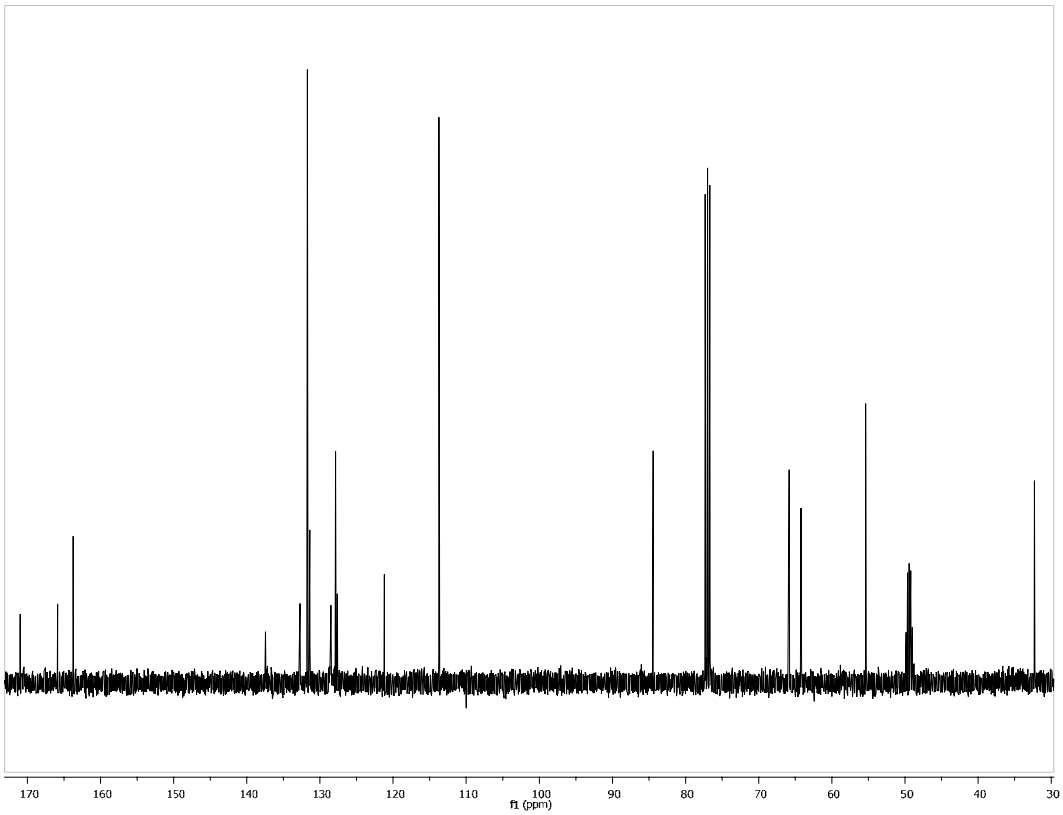
^{1}H and ^{13}C spectra of **12j-*E***



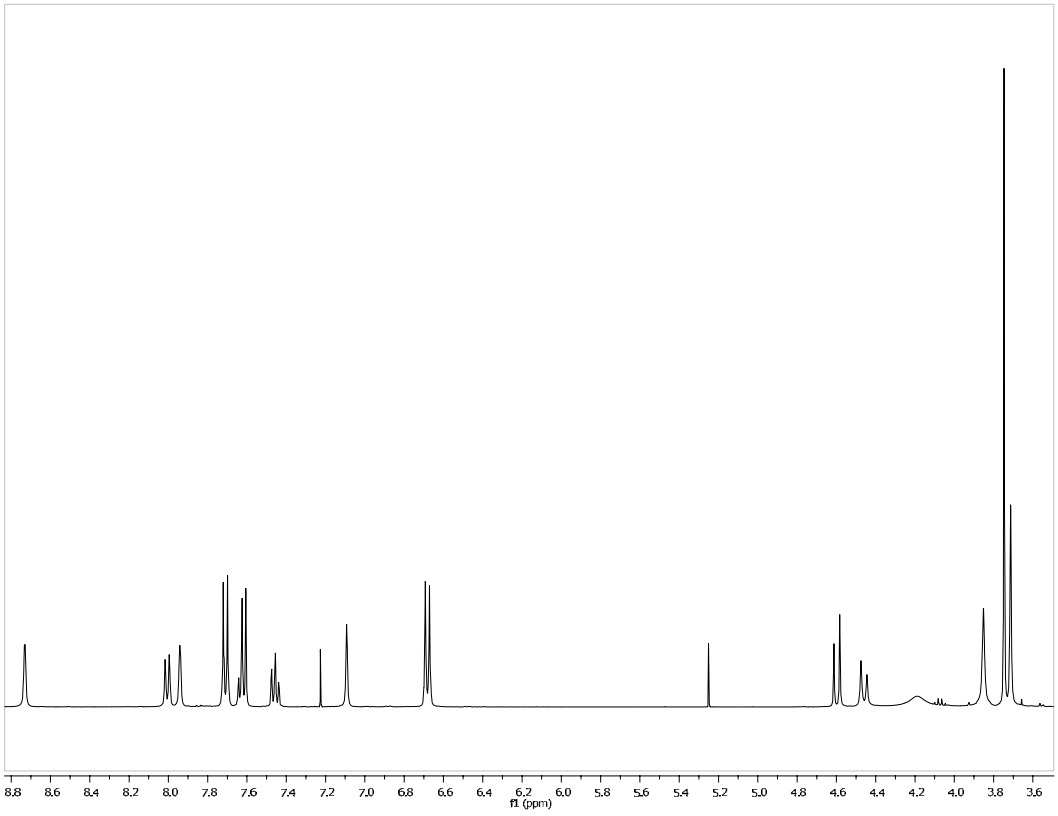


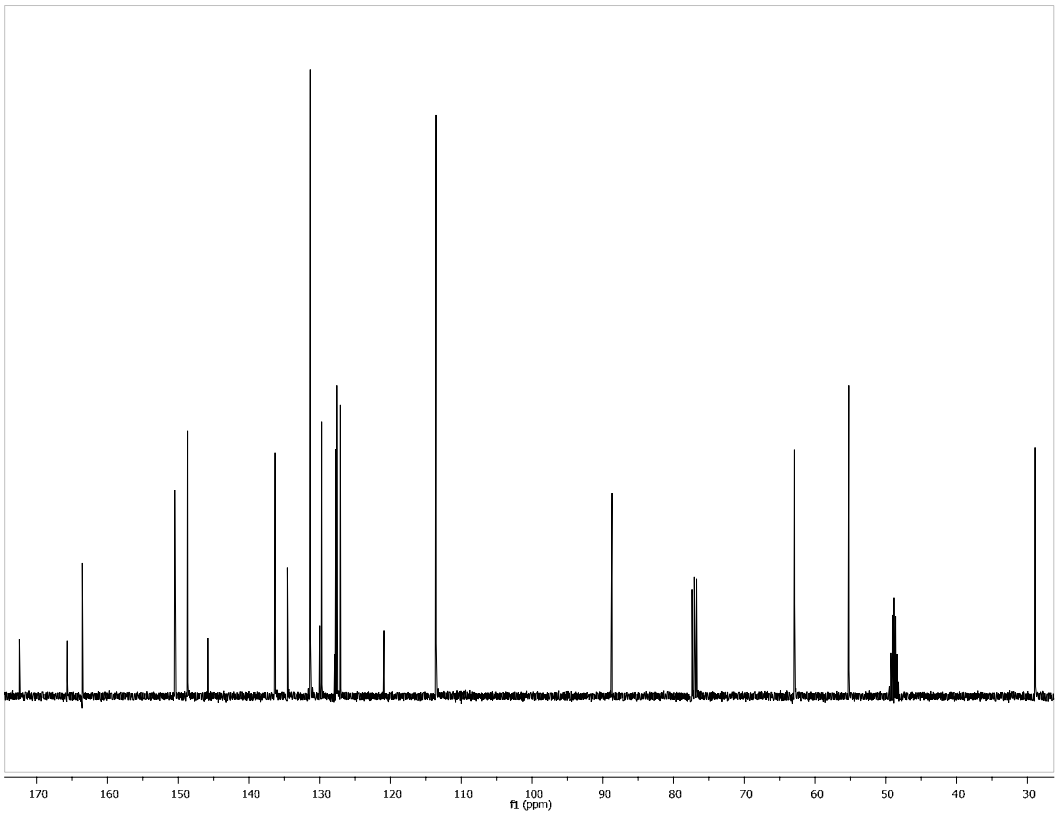
^{1}H and ^{13}C spectra of **12j-*Z***



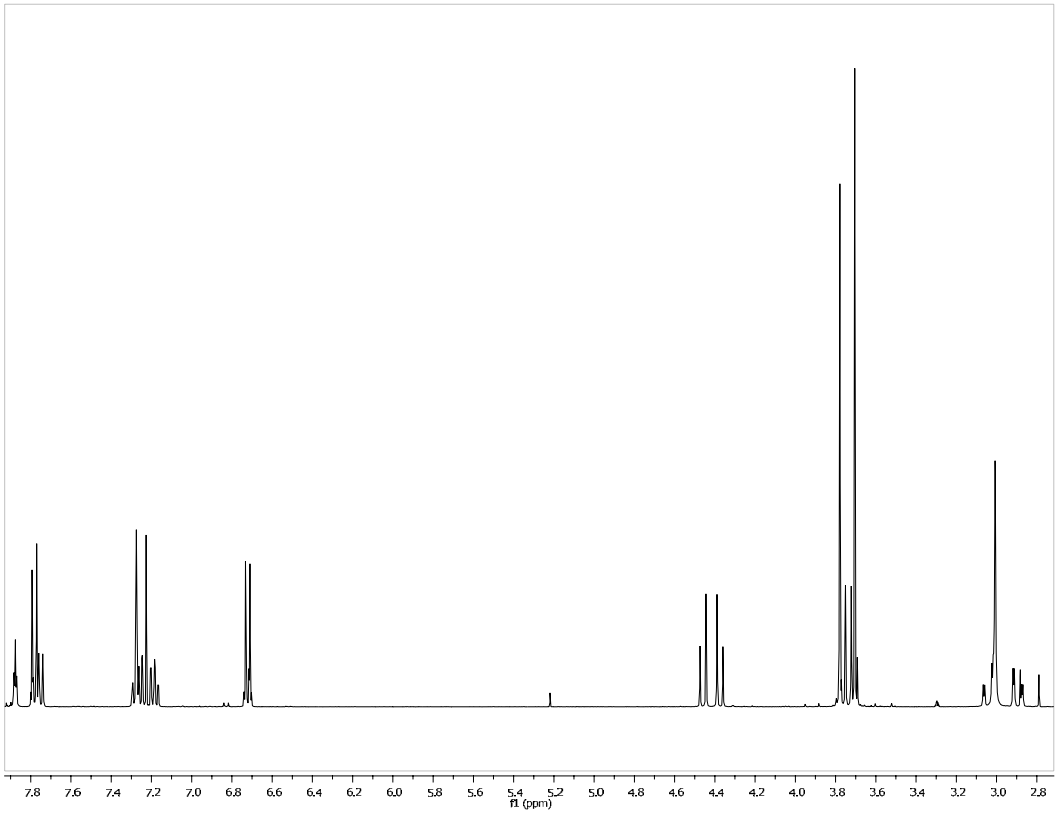


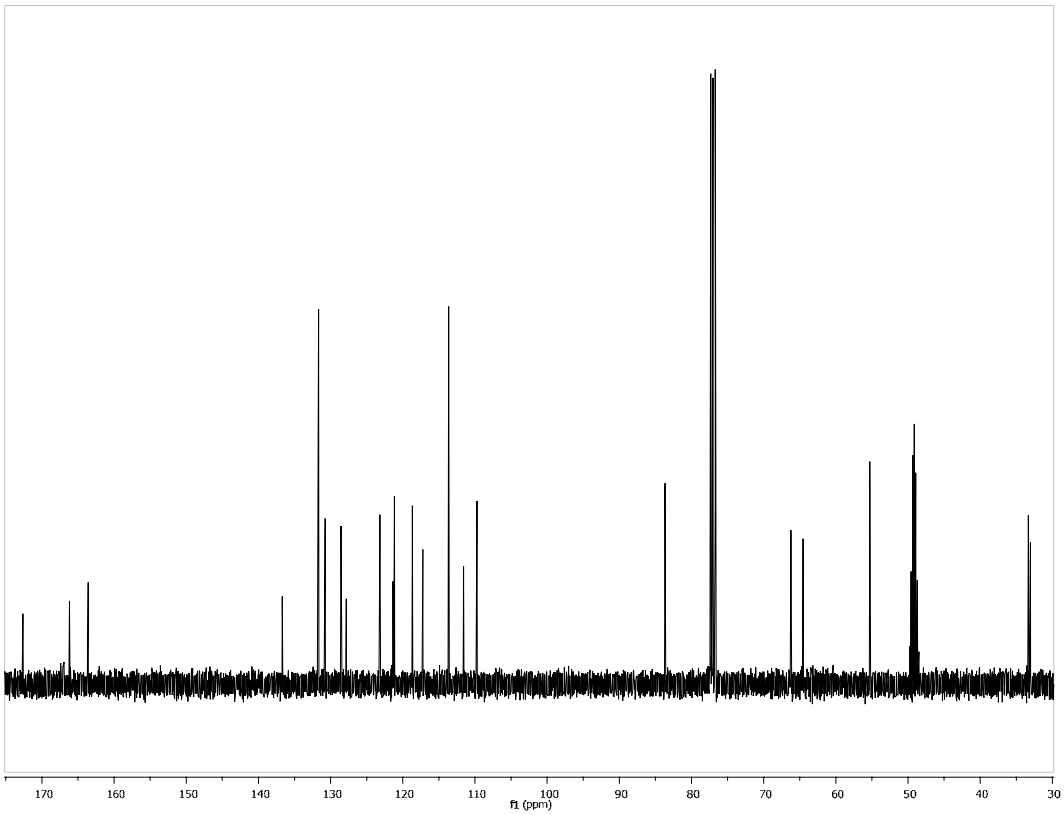
^{1}H and ^{13}C spectra of **12k-*E***



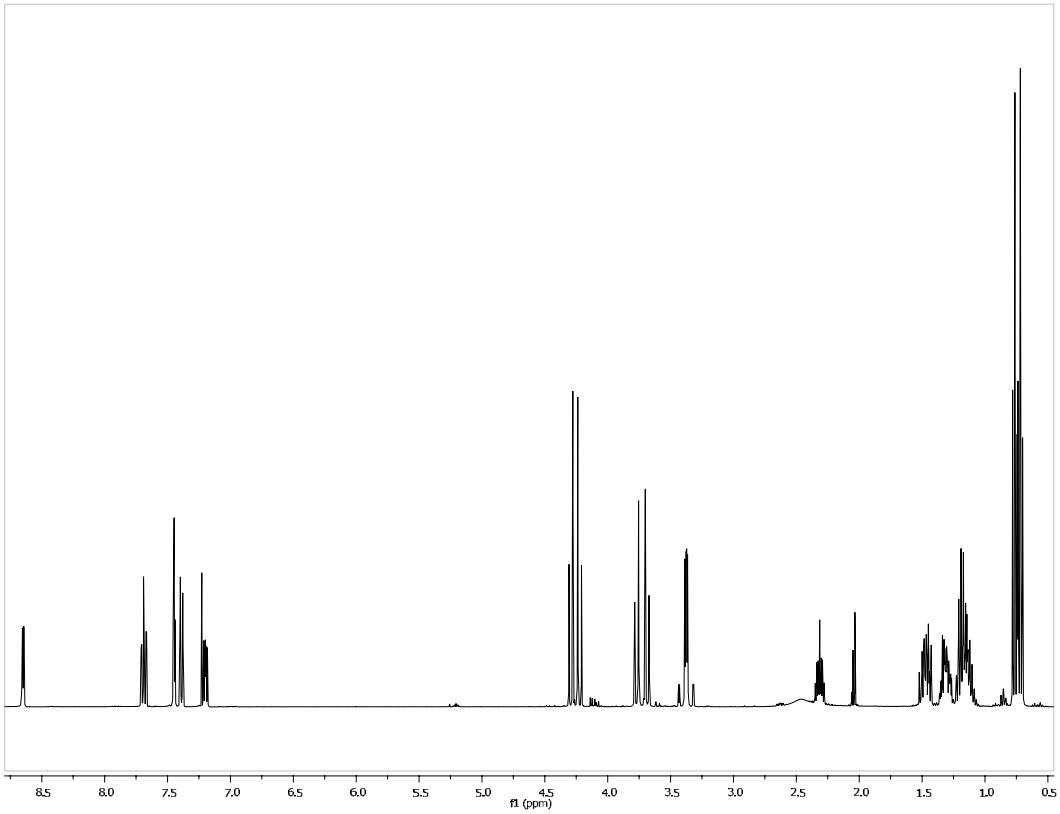


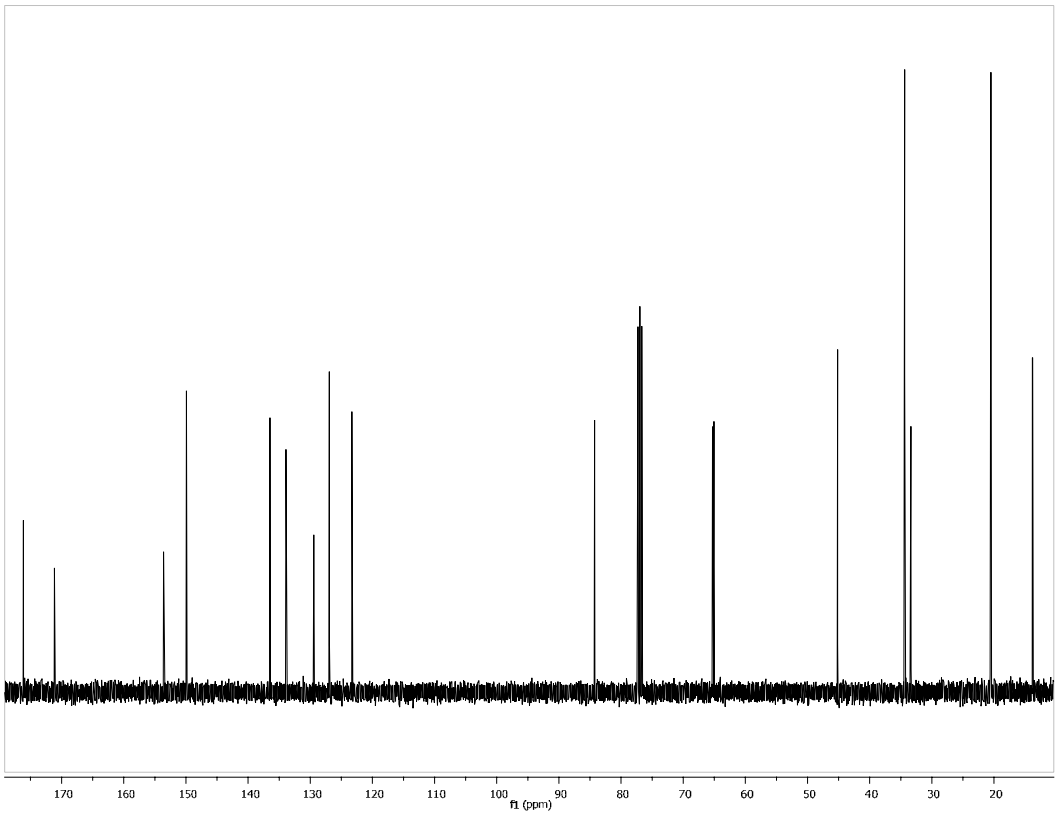
^{1}H and ^{13}C spectra of **12k-*Z***



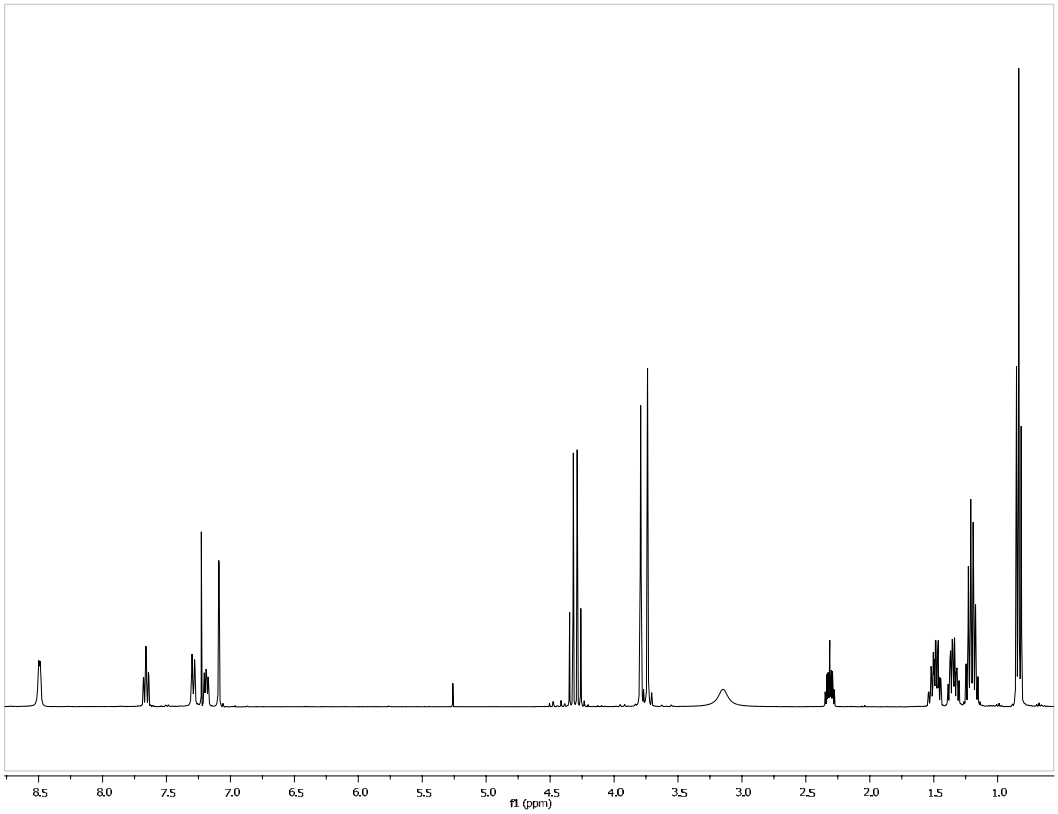


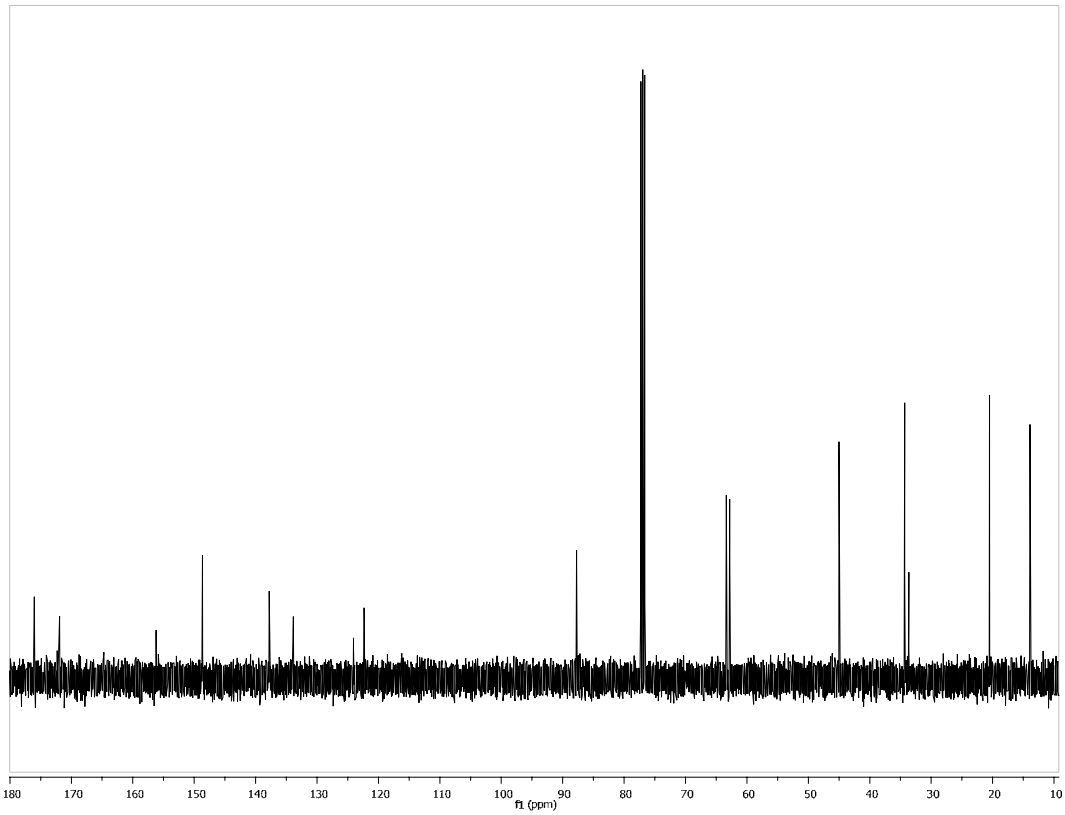
^{1}H and ^{13}C spectra of **12l-*E***



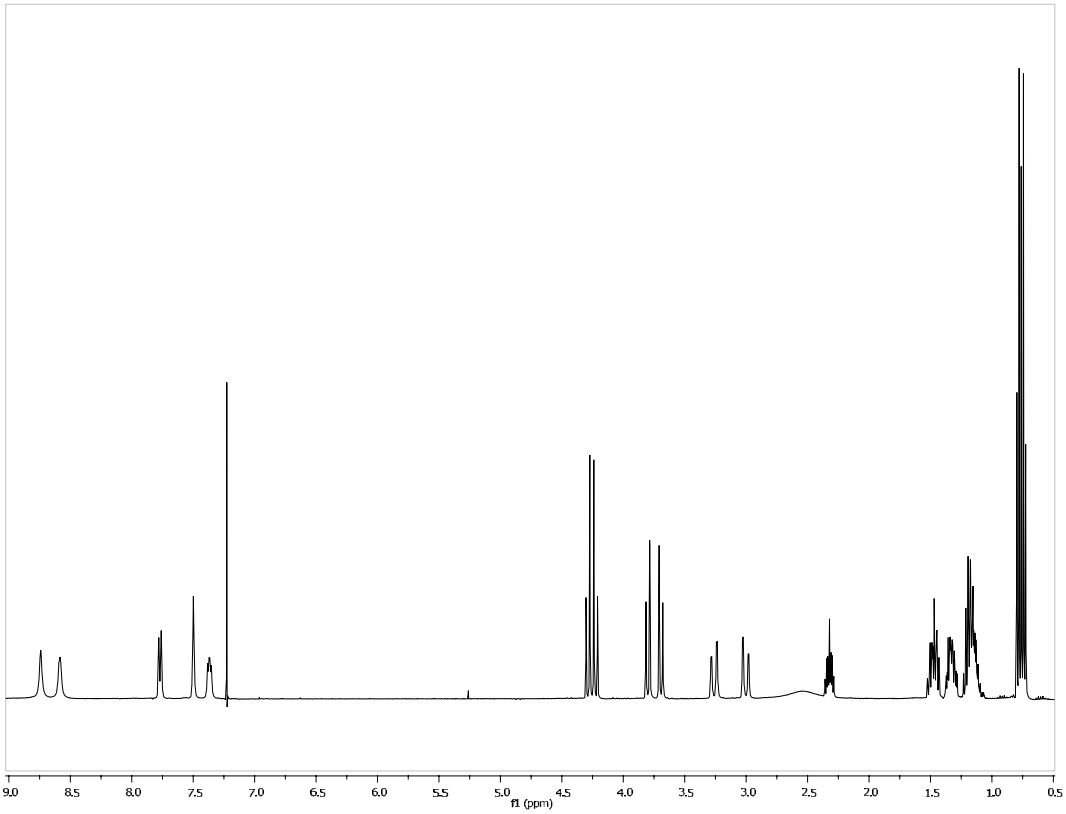


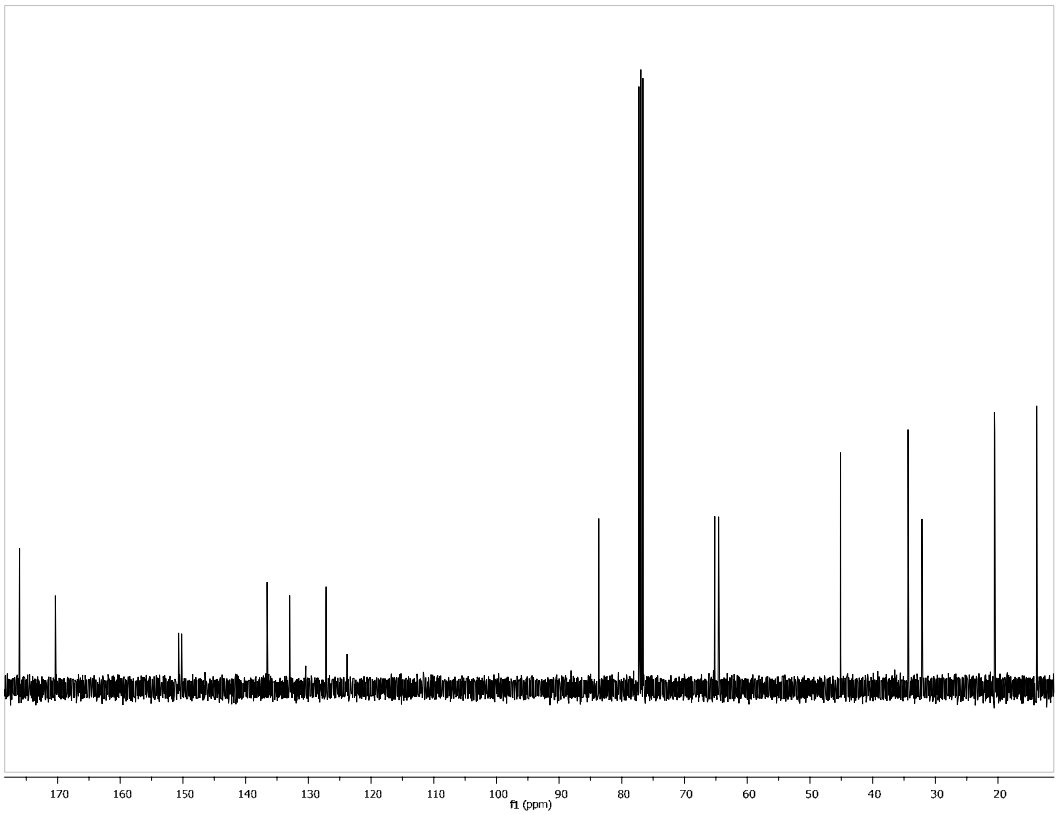
^{1}H and ^{13}C spectra of **12m-*E***



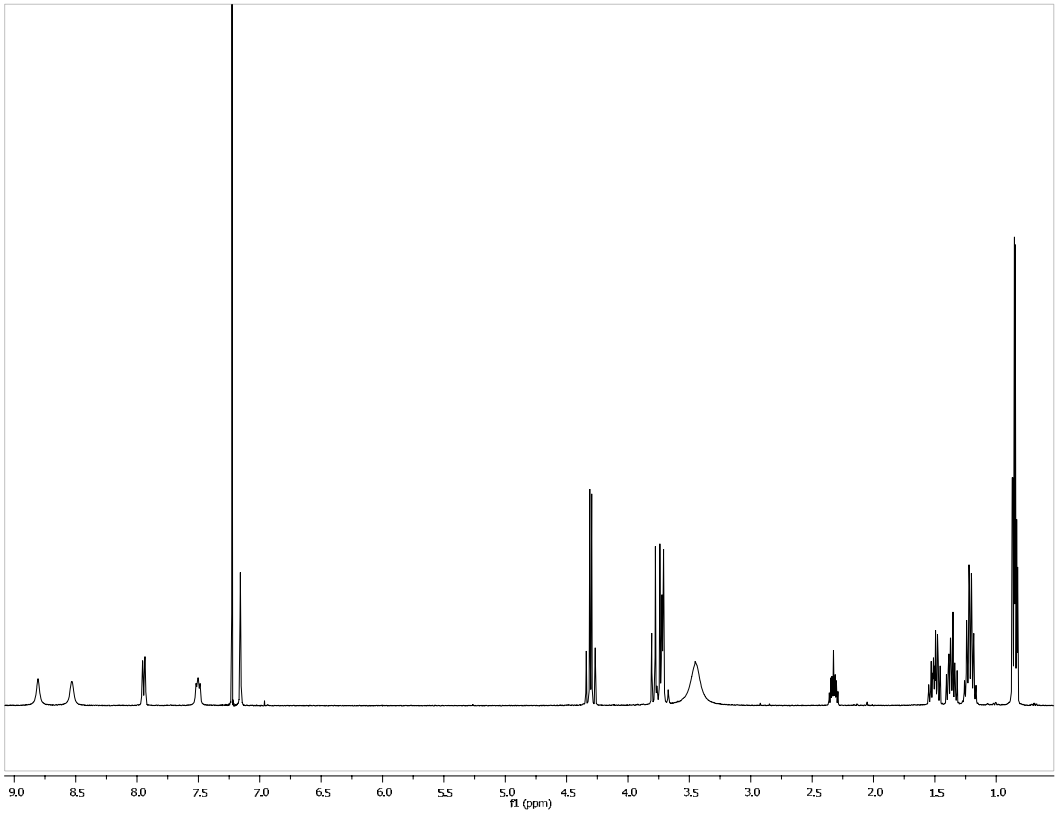


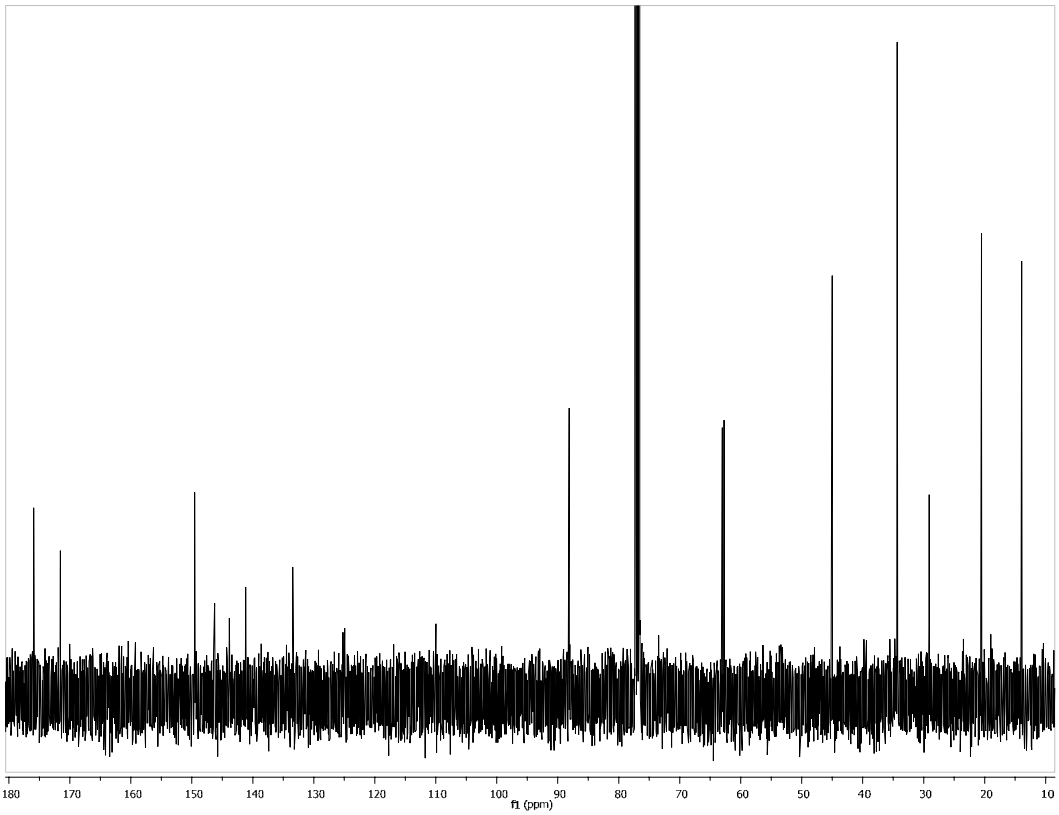
^{1}H and ^{13}C spectra of **12m-*Z***





^{1}H and ^{13}C spectra of **12n-*E***





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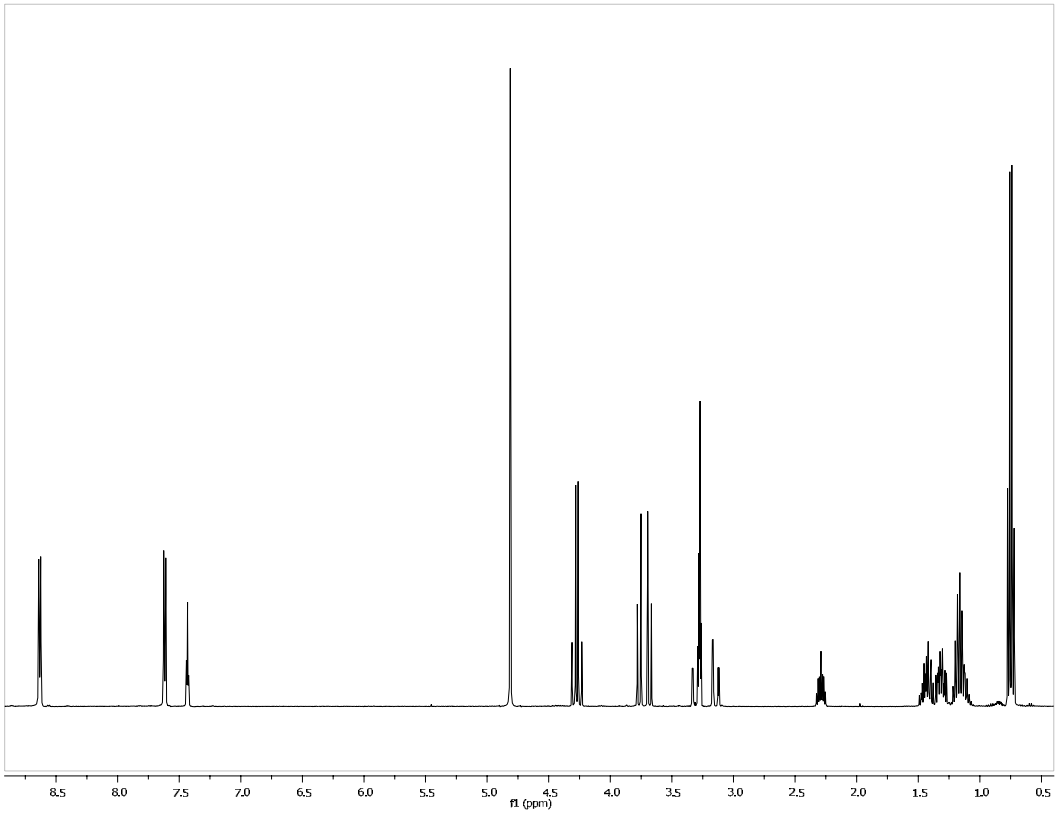
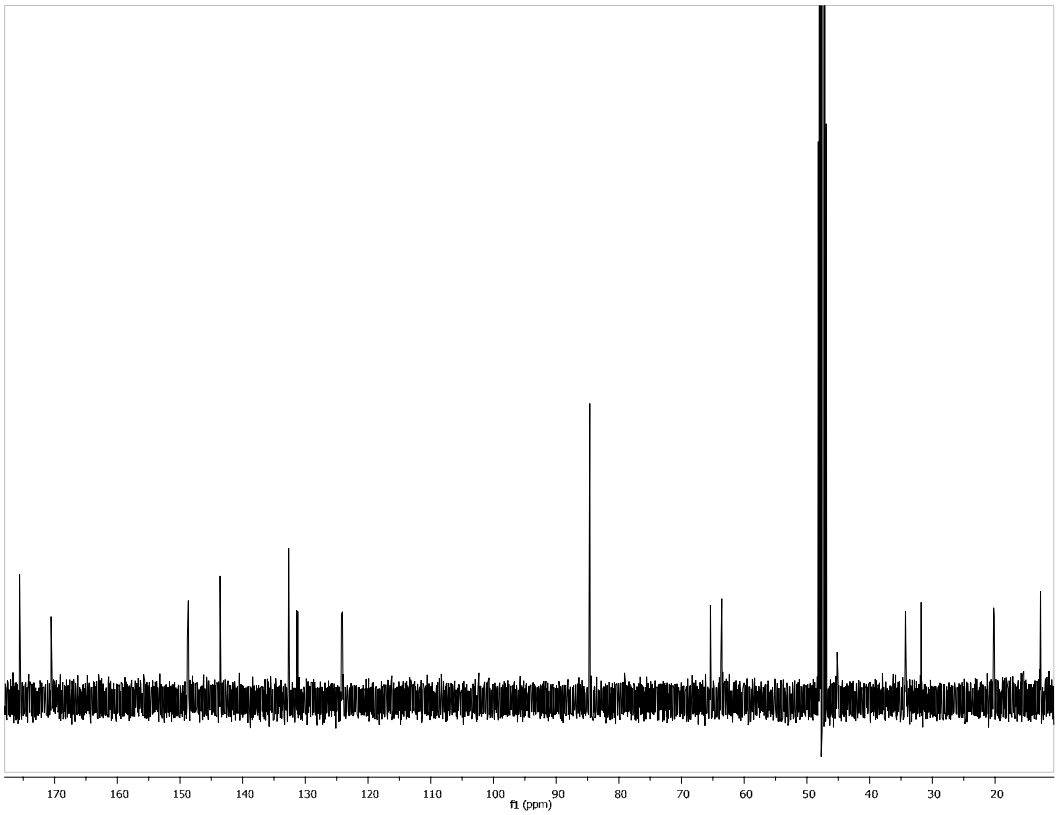
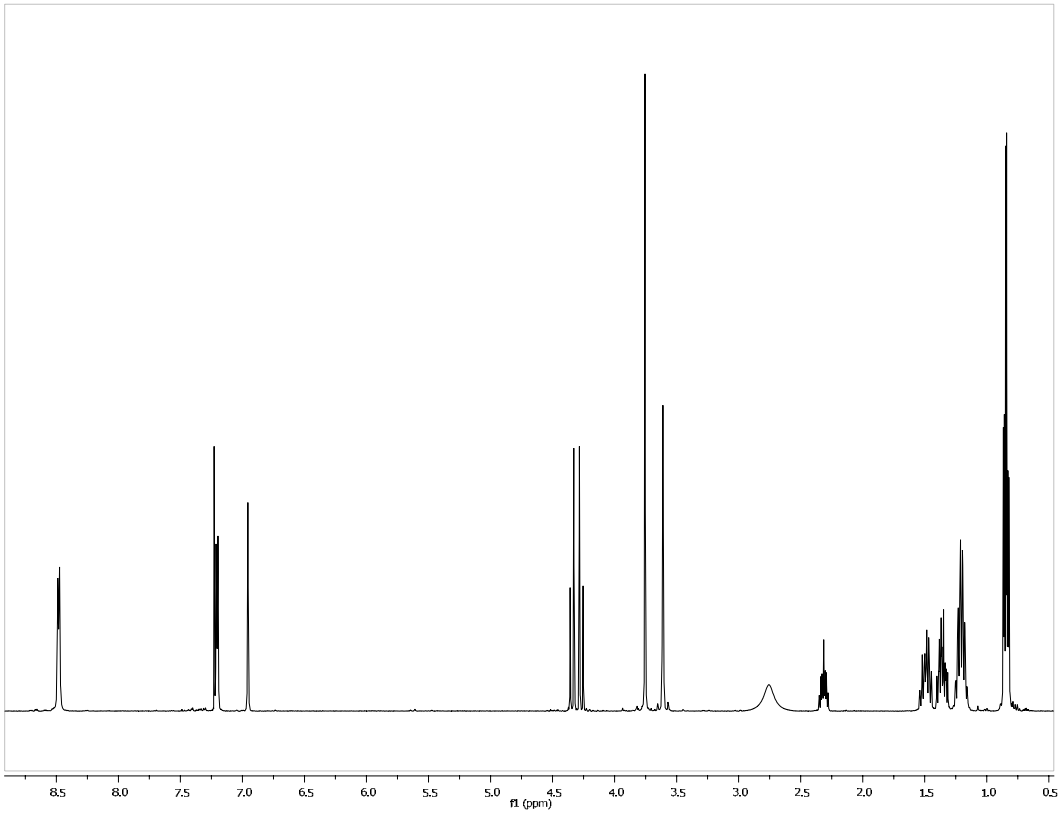
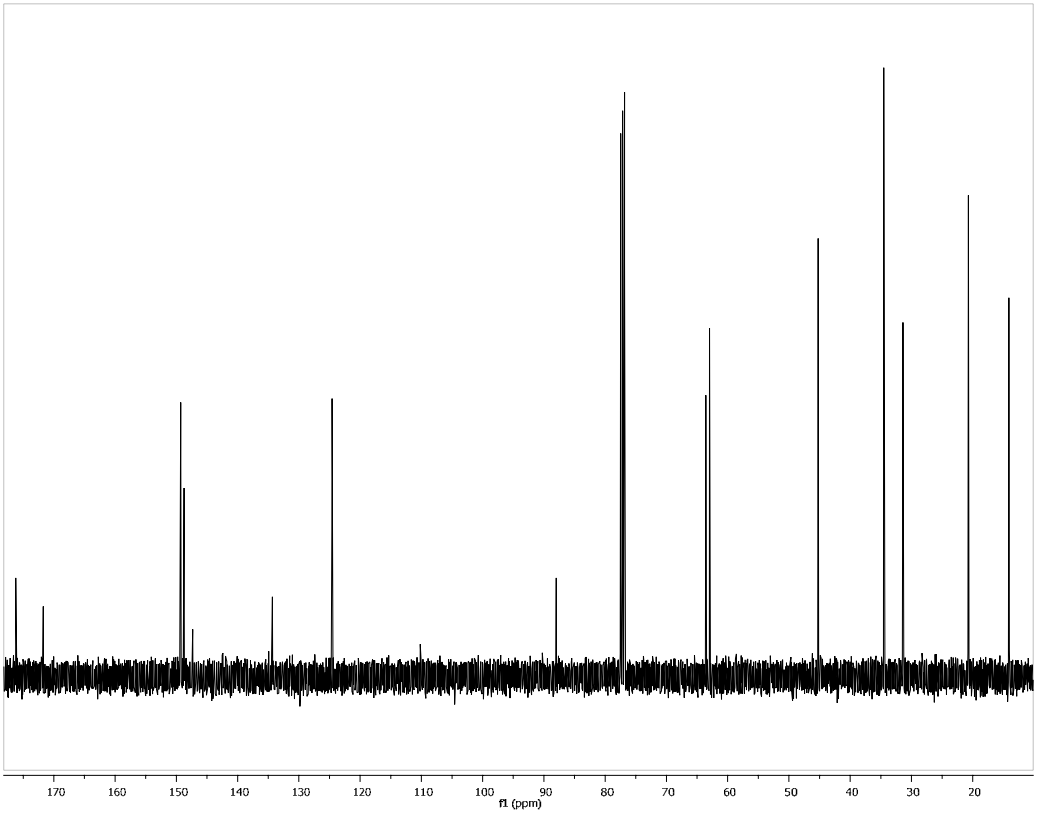


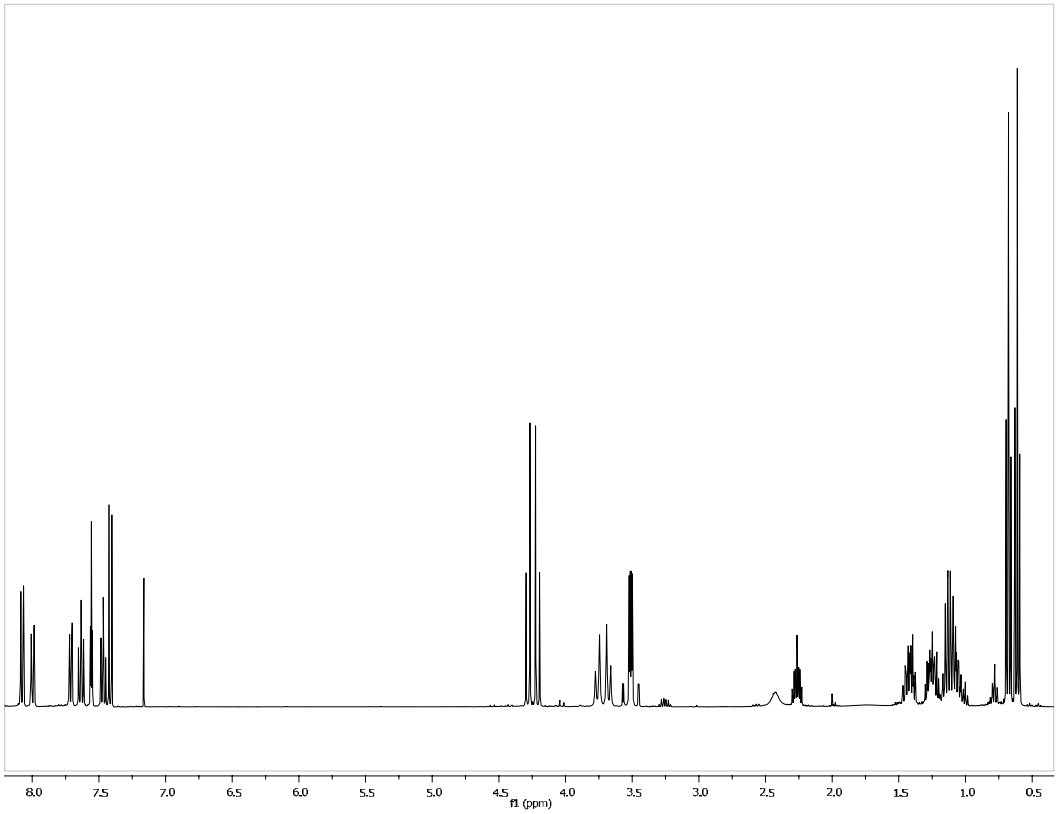


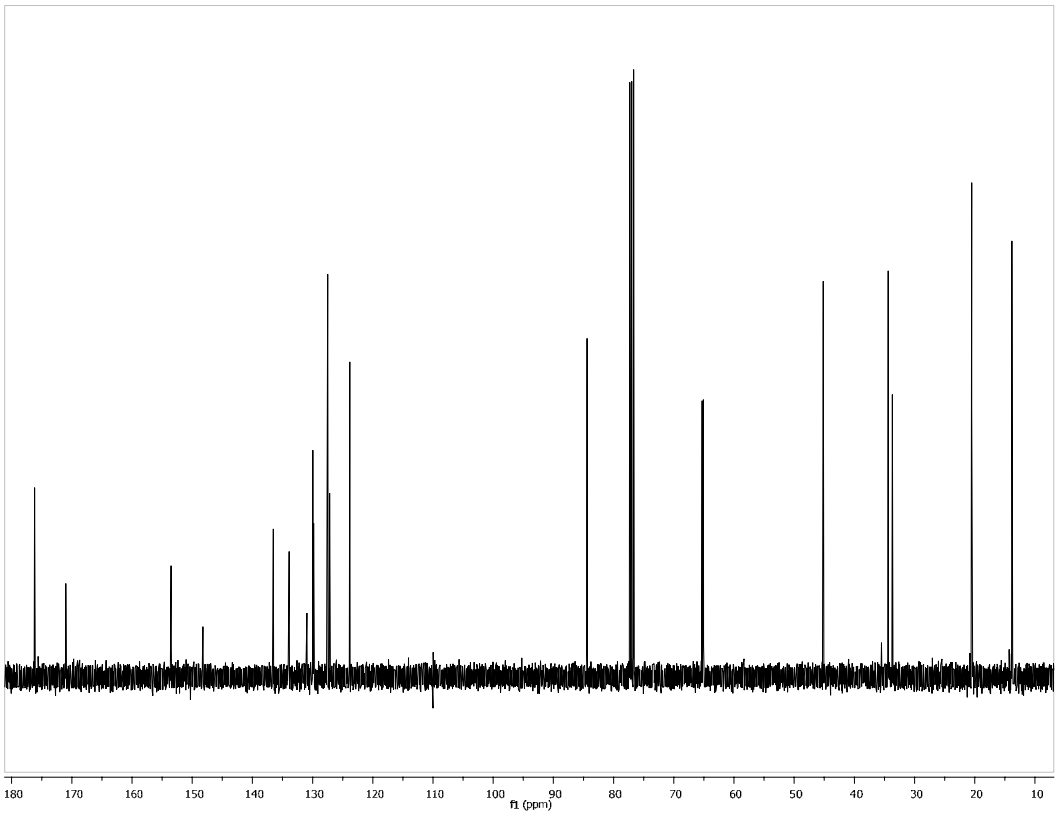
^{1}H and ^{13}C spectra of **12o-*E***



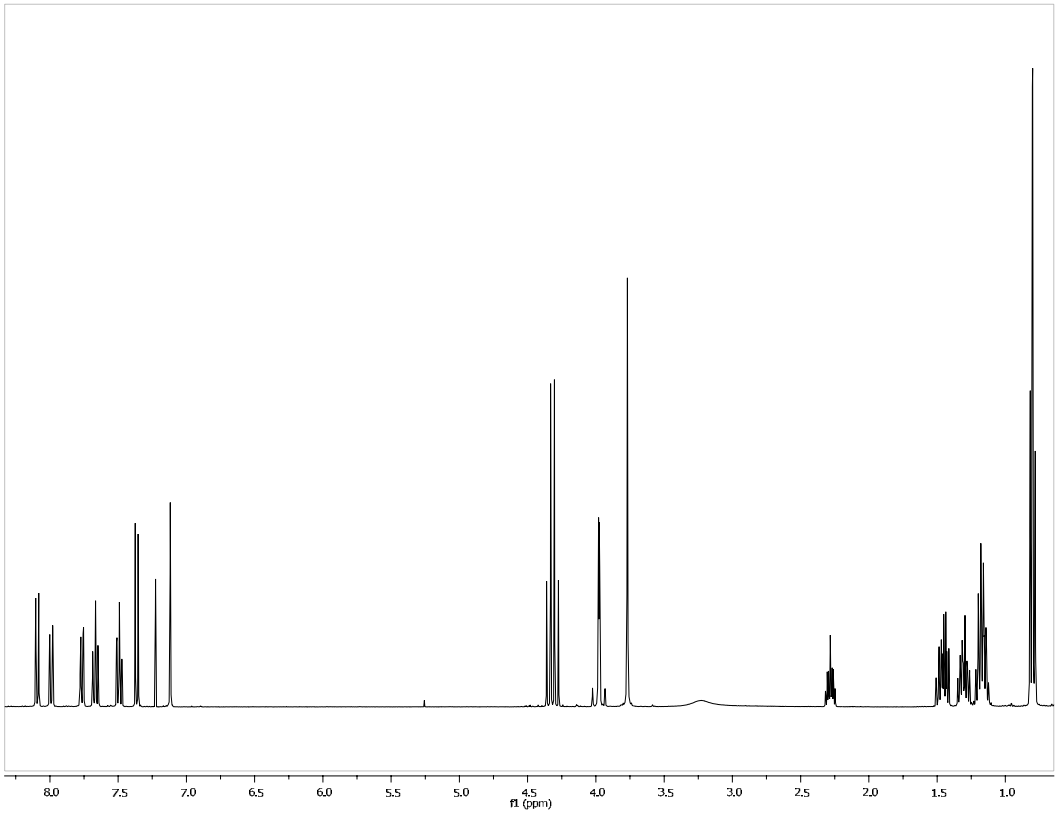


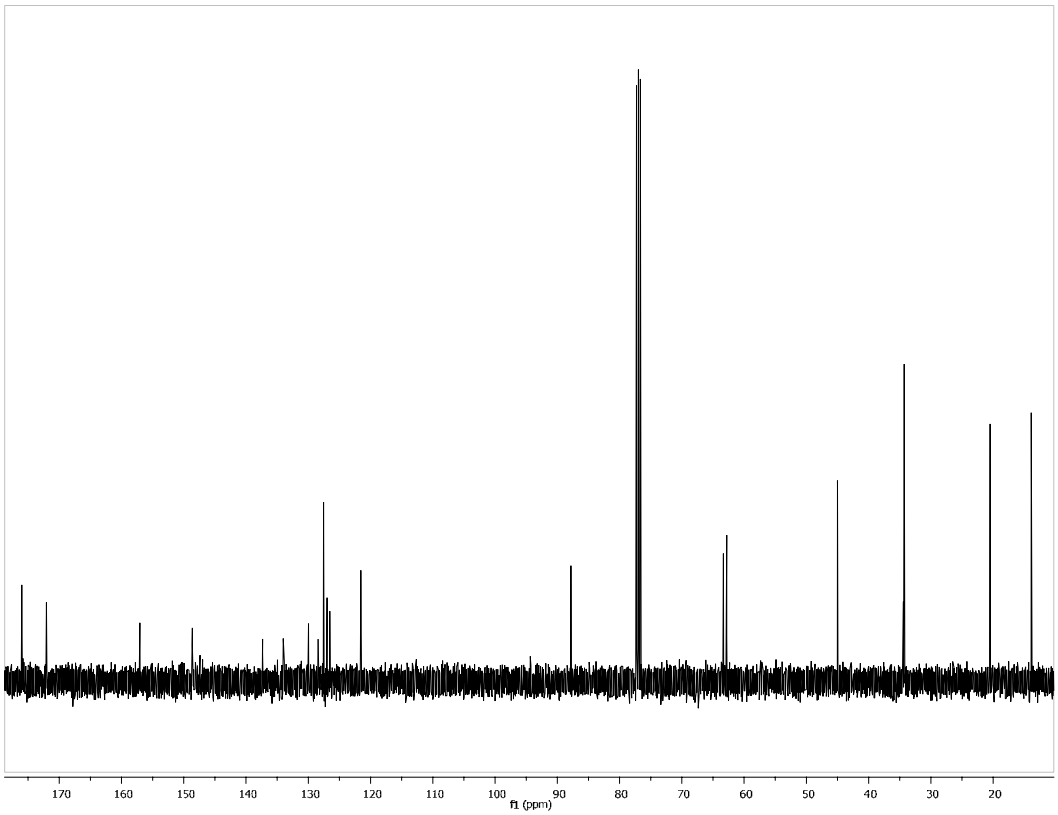
^{1}H and ^{13}C spectra of **12o-*Z***



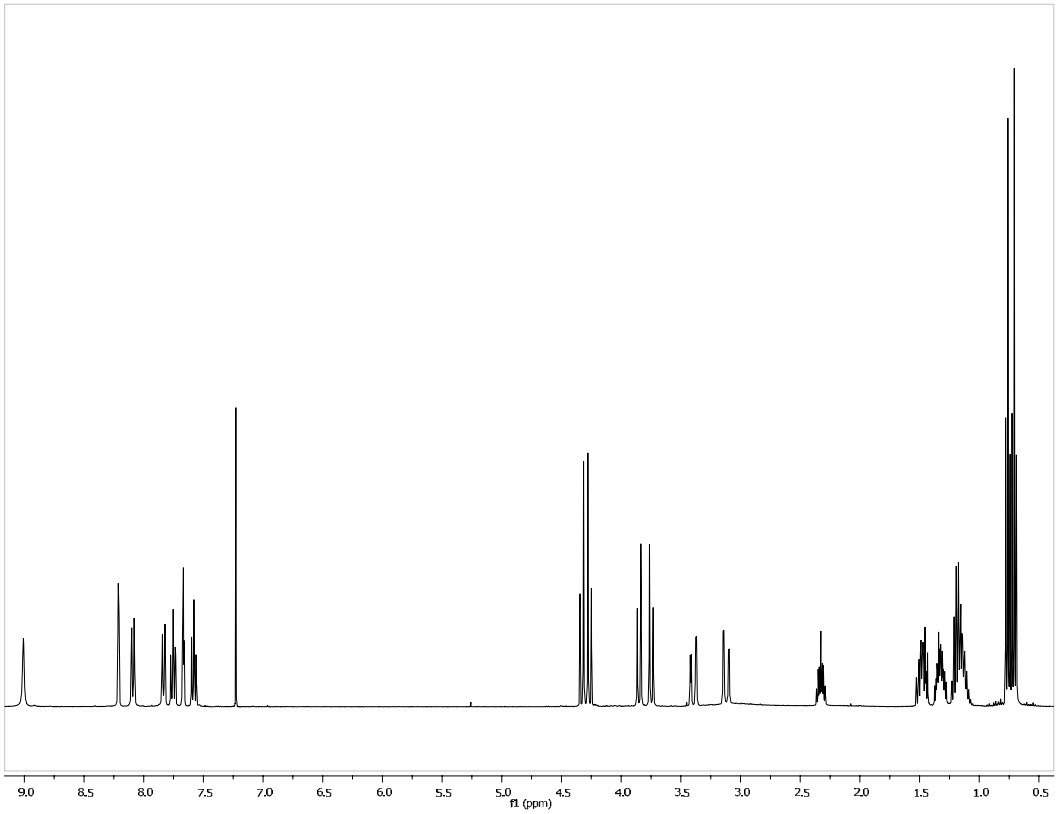


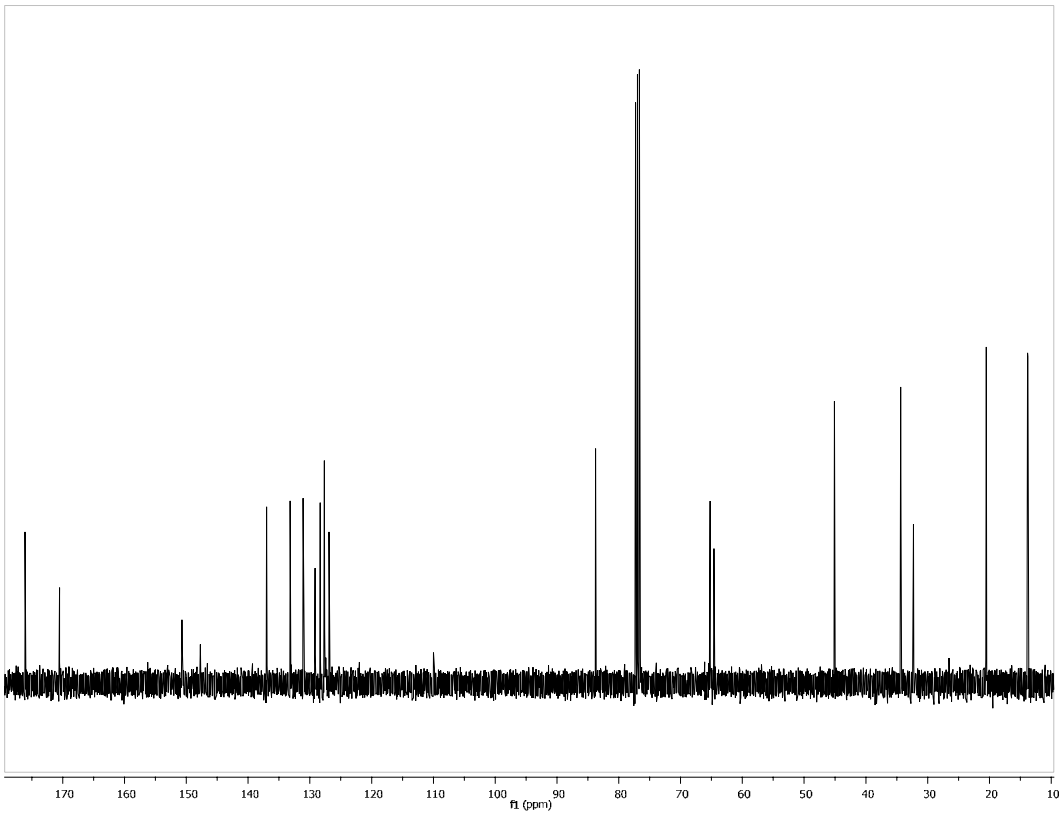
^{1}H and ^{13}C spectra of **12p-*E***



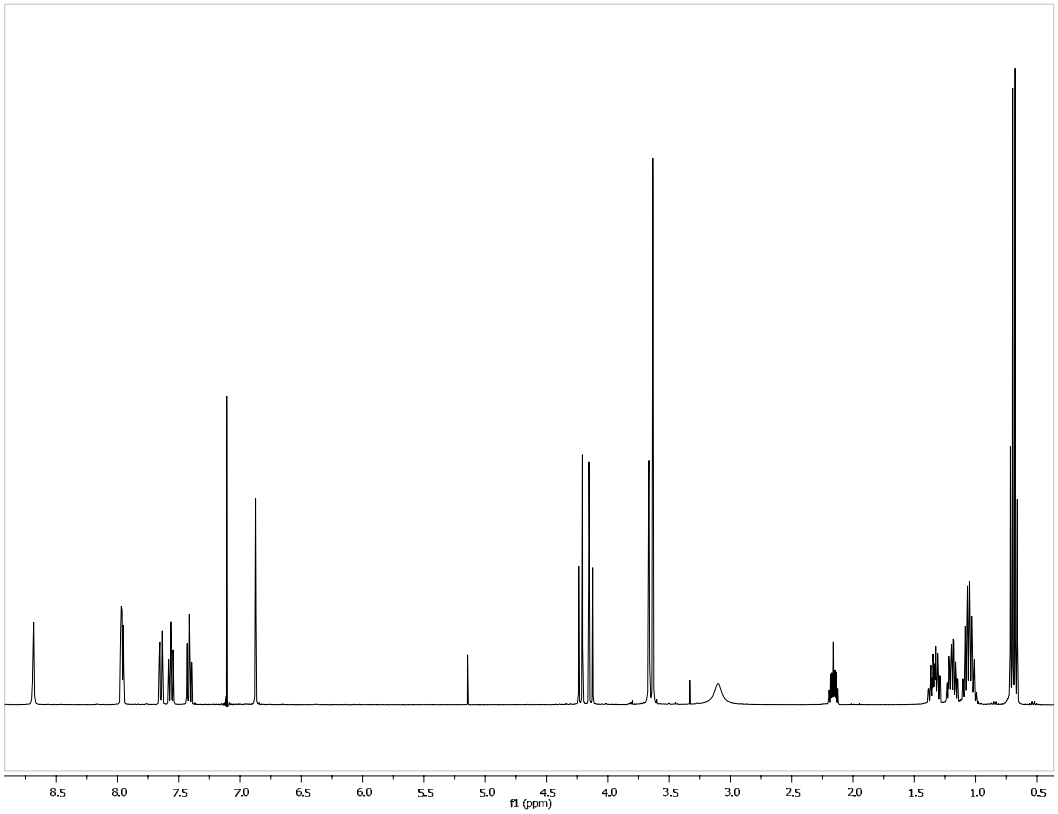


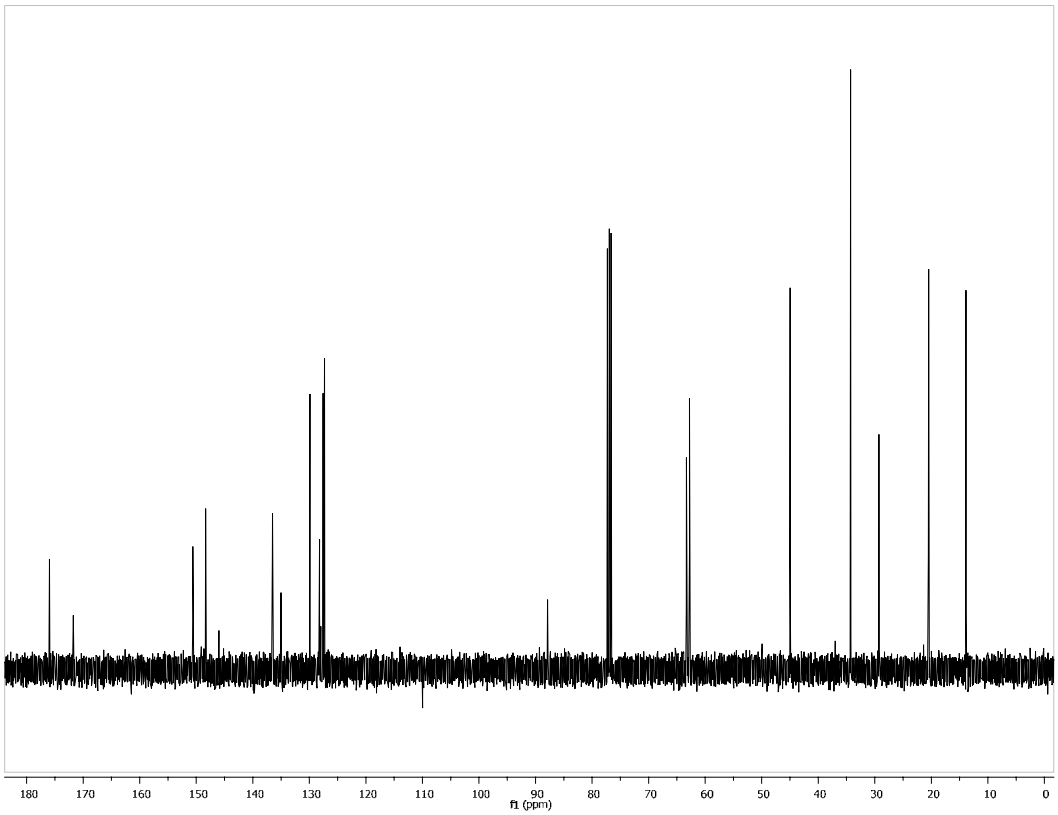
^{1}H and ^{13}C spectra of **12p-*Z***



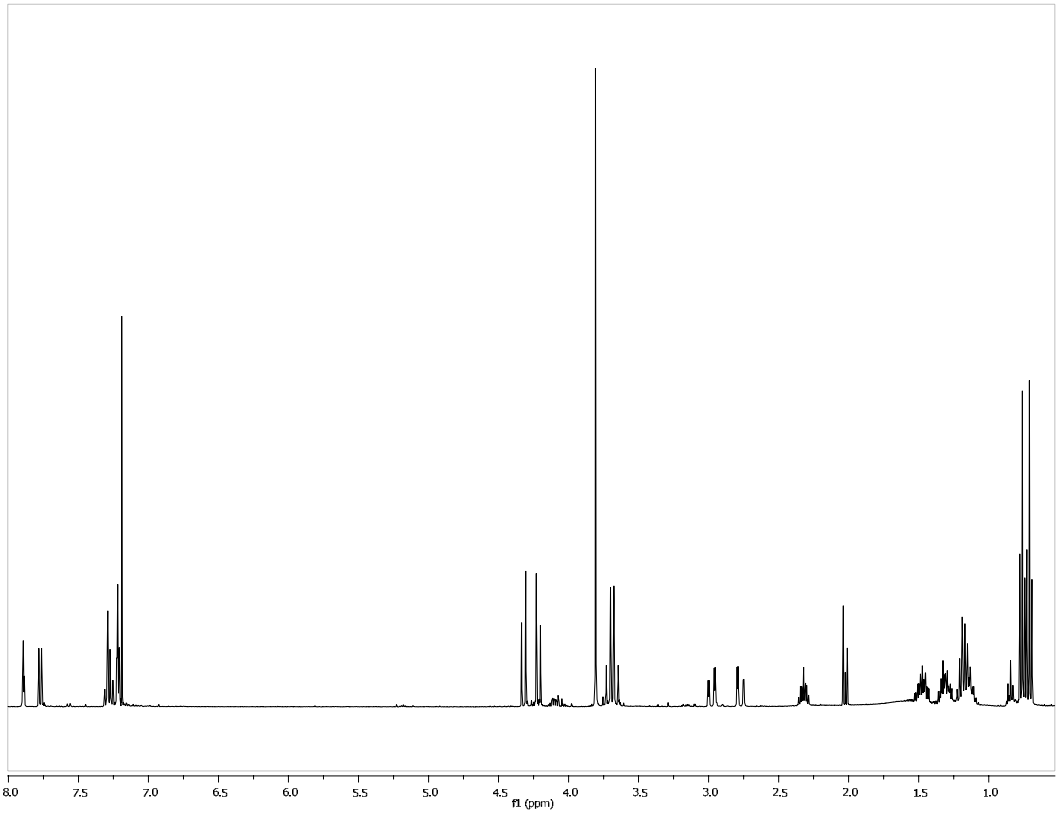


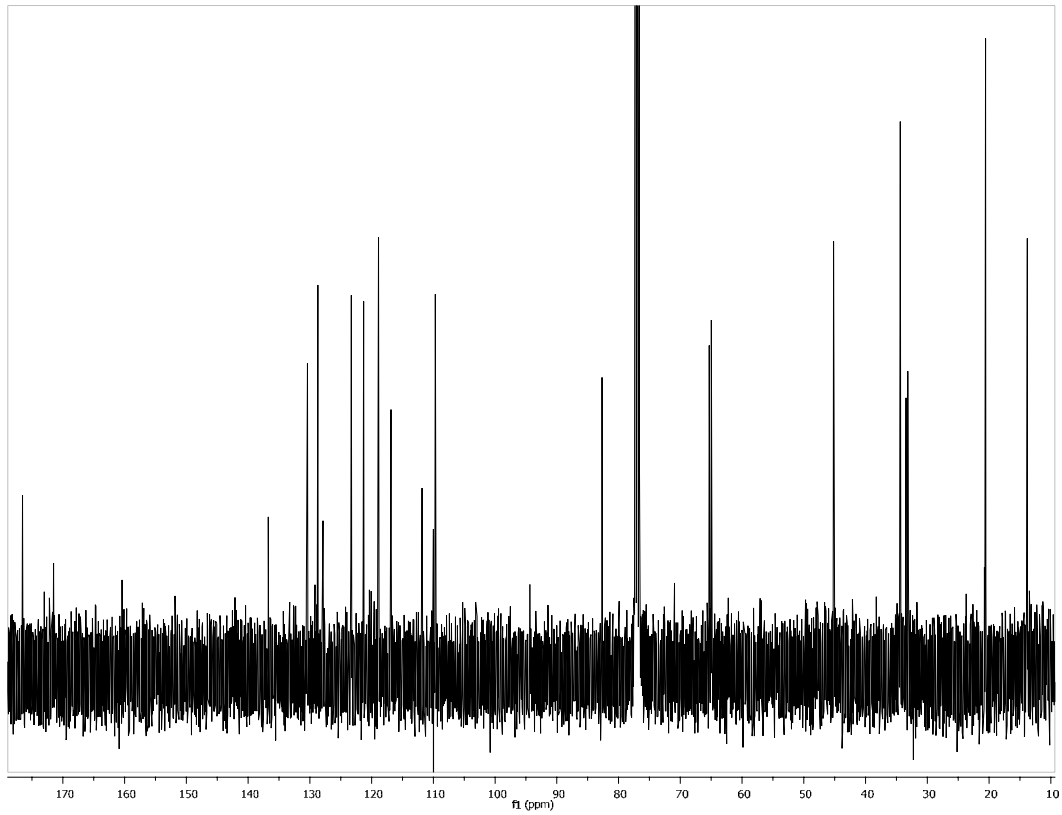
^{1}H and ^{13}C spectra of **12q-*E***



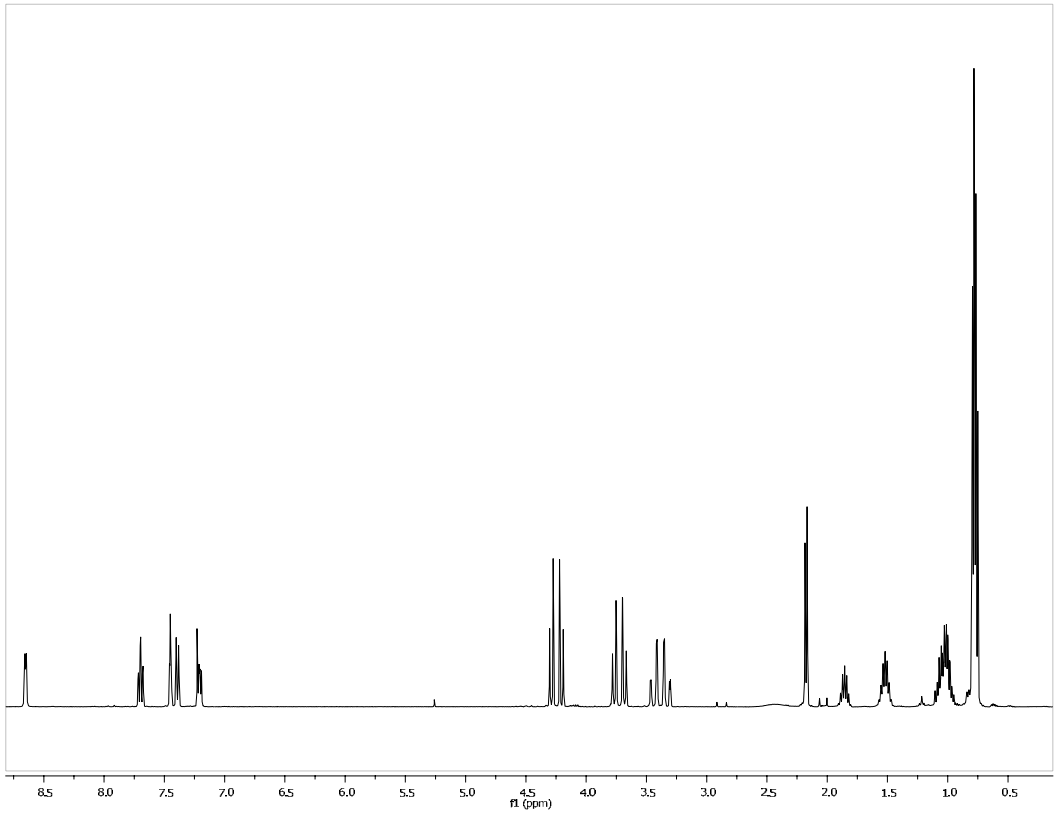


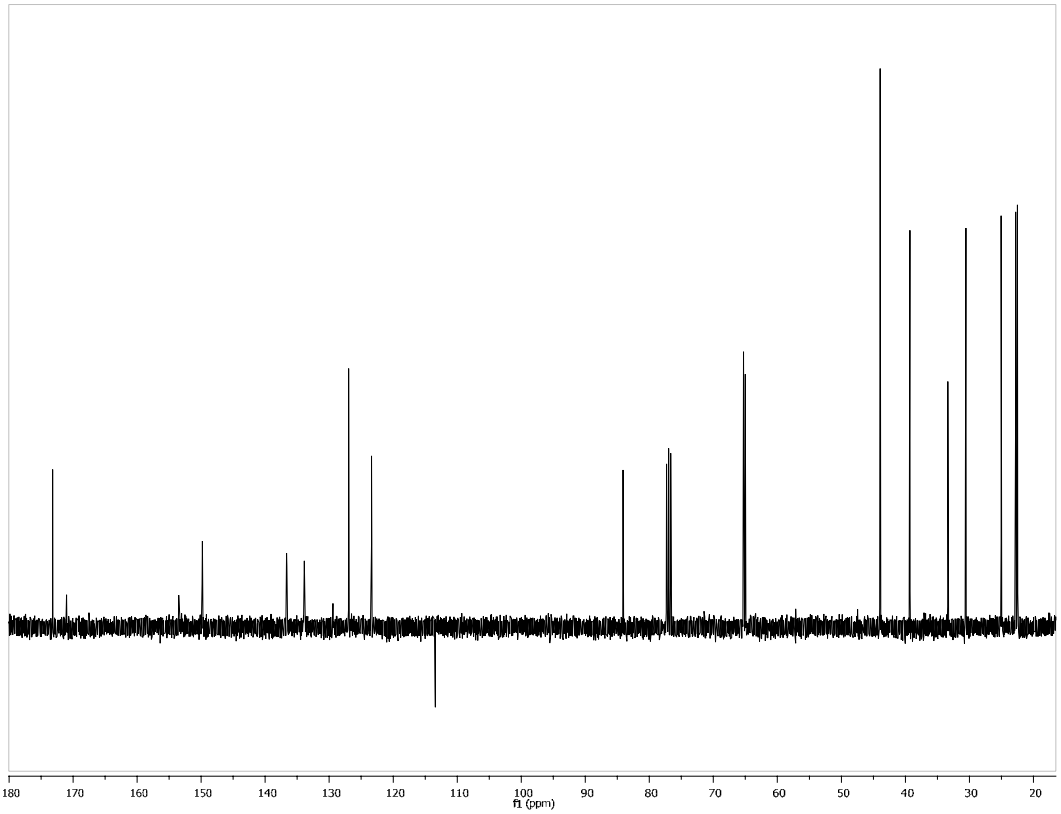
^{1}H and ^{13}C spectra of **12q-*Z***



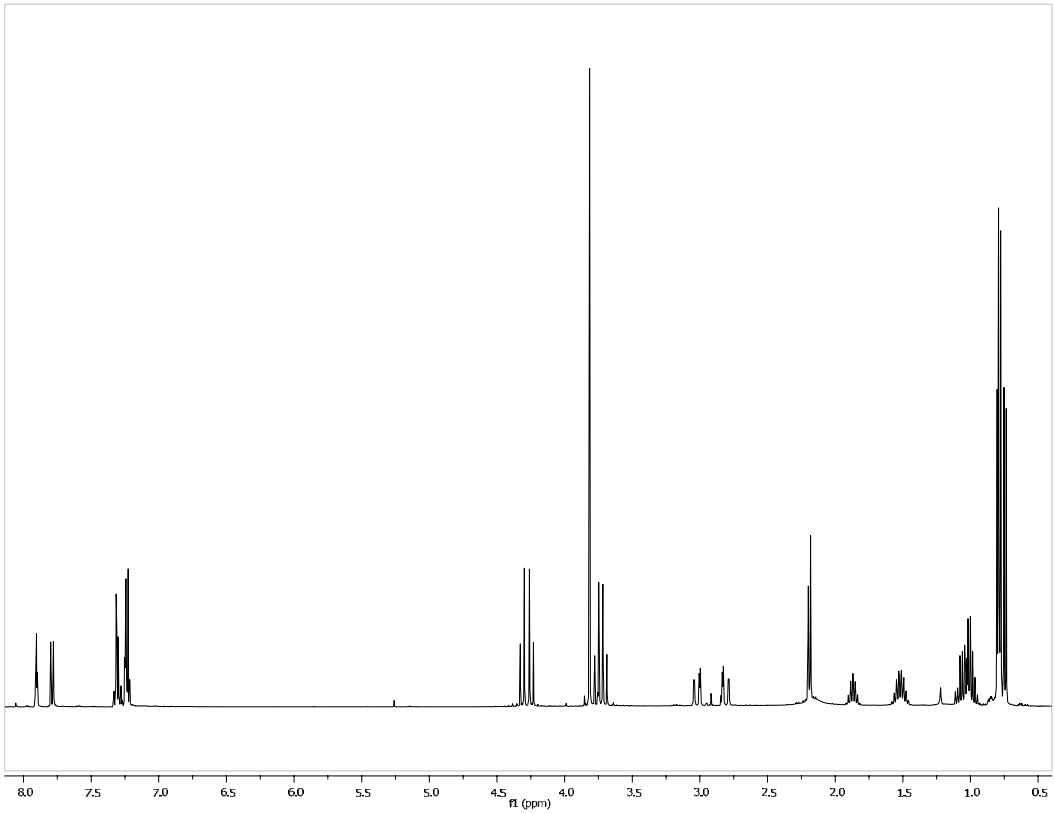


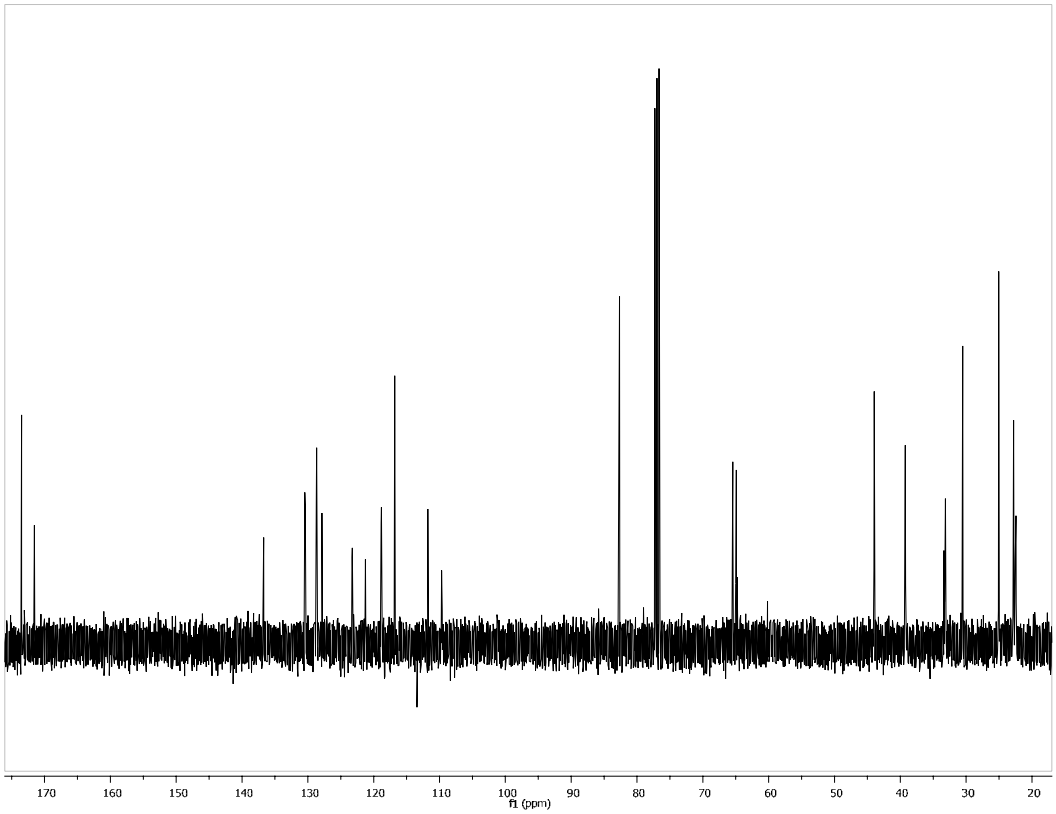
^{1}H and ^{13}C spectra of **12r-*E***





^{1}H and ^{13}C spectra of **12s-*E***





^{1}H and ^{13}C spectra of **12t-*E***