Supplementary Data

Facile Synthesis of 5-aryl-*N*-(pyrazin-2-yl)thiophene-2-carbox-amides via Suzuki Cross-Coupling Reactions, Their Electronic and Nonlinear Optical Properties through DFT Calculations

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Table S1: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4b

Compound **4b**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.38	10.59	-1.21
4	N	-	-	-
5	CH	8.47	8.44	0.03
6	CH	8.42	8.42	0.00
2'	C	-	-	-
3'	CH	8.25	7.22	1.03
4'	CH	8.03	6.77	1.26
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.74	7.58	0.16
3"	C	-	-	
4"	C	-	-	-
5"	CH	7.69	7.55	0.14
6"	CH	7.72	7.24	0.48
Mean Absolute Error (MAE) = 0.18				
Root Mean Square Error (RMSE) = 0.42				

Table S2: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4c

Compound **4c**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.42	10.64	-1.22
4	N	-	-	-
5	CH	8.17	8.44	-0.27
6	CH	8.45	8.42	0.03
2'	C	-	-	-
3'	CH	7.90	7.26	0.64
4'	CH	7.86	6.82	1.04
5'	C	-	-	-
1"	C	-	-	-
2"	CH	8.49	7.85	0.64
3"	C	-	-	-
4"	CH	7.76	7.89	-0.13
5"	CH	7.56	7.54	0.02
6"	CH	7.62	7.62	0.00
Mean Absolute Error (MAE) = 0.17				
Root Mean Square Error (RMSE) = 0.38				

Table S3: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4d

Compound **4d**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.39	10.57	-1.18
4	N	-	-	-
5	CH	8.41	8.43	-0.02
6	CH	8.47	8.42	0.05
2'	C	-	-	-
3'	CH	8.25	7.22	1.03
4'	CH	7.64	6.72	0.92
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.51	7.39	0.12
3"	CH	7.77	7.41	0.36
4"	C	-	-	-
5"	CH	7.77	7.41	0.36
6"	CH	7.51	7.39	0.12
Mean Absolute Error (MAE) = 0.17				
Root Mean Square Error (RMSE) = 0.38				

Table S4: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4e

Compound **4e**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.38	10.63	-1.25
4	N	-	-	-
5	CH	8.42	8.44	-0.02
6	CH	8.48	8.42	0.06
2'	C	-	-	-
3'	CH	8.25	7.22	1.04
4'	CH	8.01	6.77	1.25
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.76	7.57	0.19
3"	C	-	-	-
4"	C	-	-	-
5"	CH	7.51	7.27	0.24
6"	CH	7.68	7.32	0.36
Mean Absolute Error (MAE) = 0.18				
Root Mean Square Error (RMSE) = 0.42				

Table S5: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4f

Compound **4f**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.40	10.63	-1.23
4	N	-	-	-
5	CH	8.39	8.40	-0.01
6	CH	8.44	8.40	0.04
2'	C	-	-	-
3'	CH	8.23	7.20	1.03
4'	CH	7.52	7.14	0.38
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.32	7.37	-0.05
3"	C	-	-	-
4"	CH	6.97	7.15	-0.18
5"	C	-	-	-
6"	CH	7.32	7.35	-0.03
Mean Absolute Error (MAE) = 0.12				
Root Mean Square Error (RMSE) = 0.33				

Table S6: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4g

Compound **4g**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.33	10.58	-1.25
4	N	-	-	-
5	CH	8.41	8.39	0.02
6	CH	8.46	8.40	0.06
2'	C	-	-	-
3'	CH	8.26	7.18	1.08
4'	CH	8.22	6.65	1.57
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.66	7.42	0.24
3"	CH	7.33	6.58	0.75
4"	C	-	-	-
5"	CH	7.33	7.19	0.14
6"	CH	7.66	7.43	0.23
Mean Absolute Error (MAE) = 0.22				
Root Mean Square Error (RMSE) = 0.49				

Table S7: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4h

Compound **4h**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.38	10.58	-1.20
4	N	-	-	-
5	CH	8.41	8.44	-0.03
6	CH	8.48	8.42	0.06
2'	C	-	-	-
3'	CH	8.26	7.25	1.01
4'	CH	7.94	6.82	1.12
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.24	7.57	-0.33
3"	CH	7.78	8.33	-0.55
4"	C	-	-	-
5"	CH	7.78	8.54	-0.76
6"	CH	7.24	7.52	-0.28
Mean Absolute Error (MAE) = 0.22				
Root Mean Square Error (RMSE) = 0.44				

Table S8: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4i

Compound **4i**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.38	10.57	-1.19
4	N	-	-	-
5	CH	8.41	8.40	0.01
6	CH	8.47	8.40	0.07
2'	C	-	-	-
3'	CH	8.24	7.19	1.05
4'	CH	7.70	6.66	1.04
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.70	7.33	0.37
3"	CH	7.33	6.87	0.46
4"	C	-	-	-
5"	CH	7.33	7.20	0.13
6"	CH	7.60	7.30	0.30
Mean Absolute Error (MAE) = 0.19				
Root Mean Square Error (RMSE) = 0.41				

Table S9: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4j

Compound **4j**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.37	10.52	-1.15
4	N	-	-	-
5	CH	8.26	8.44	-0.18
6	CH	8.47	8.43	0.04
2'	C	-	-	-
3'	CH	7.76	7.25	0.51
4'	CH	7.61	6.82	0.79
5'	C	-	-	-
1"	C	-	-	-
2"	CH	7.52	6.92	0.60
3"	C	-	-	-
4"	CH	7.26	6.95	0.31
5"	C	-	-	-
6"	CH	7.52	6.95	0.57
Mean Absolute Error (MAE) = 0.17 Root Mean Square Error (RMSE) = 0.35				

Table S10: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4k

Compound **4k**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.42	10.56	-1.14
4	N	-	-	-
5	CH	8.44	8.43	0.01
6	CH	8.49	8.41	0.08
2'	C	-	-	-
3'	CH	8.28	7.19	1.09
4'	CH	7.52	6.73	0.79
5'	C	-	-	-
1"	C	-	-	-
2"	C	-	-	-
3"	CH	7.30	6.78	0.52
4"	CH	7.12	6.63	0.49
5"	C	-	-	-
Mean Absolute Error (MAE) = 0.17 Root Mean Square Error (RMSE) = 0.38				

Table S11: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4l

Compound **4l**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.37	10.57	-1.20
4	N	-	-	-
5	CH	8.41	8.40	0.01
6	CH	8.47	8.40	0.07
2'	C	-	-	-
3'	CH	8.18	7.15	1.04
4'	CH	7.30	6.71	0.59
5'	C	-	-	-
1"	C	-	-	-
2"	C	-	-	-
3"	CH	6.84	6.76	0.08
4"	CH	7.30	6.46	0.84
5"	C	-	-	-
Mean Absolute Error (MAE) = 0.16 Root Mean Square Error (RMSE) = 0.38				

Table S12: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4m

Compound **4m**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.09	10.56	-1.47
4	N	-	-	-
5	CH	8.49	8.48	0.01
6	CH	8.61	8.45	0.16
2'	C	-	-	-
3'	CH	7.89	7.28	0.61
4'	CH	7.71	6.85	0.86
5'	C	-	-	-
1"	C	-	-	-
2"	CH	8.02	8.01	0.01
3"	C	-	-	-
4"	CH	8.45	8.23	0.22
5"	C	-	-	-
6"	CH	8.02	8.06	-0.04
Mean Absolute Error (MAE) = 0.14 Root Mean Square Error (RMSE) = 0.37				

Table S13: Comparison of experimental and theoretical ^{1}H-NMR data of compound 4n

Compound **4n**				
Carbon No.	Carbon Type	^{1}H-NMR (δ, ppm) Experimental	^{1}H-NMR (δ, ppm) Computed	Δδ, ppm
2	C	-	-	-
3	CH	9.13	10.57	-1.44
4	N	-	-	-
5	CH	8.51	8.46	0.05
6	CH	8.54	8.44	0.10
2'	C	-	-	-
3'	CH	8.00	7.28	0.72
4'	CH	7.85	6.88	0.97
5'	C	-	-	-
1"	C	-	-	-
2"	CH	8.48	7.68	0.80
3"	C	-	-	-
4"	CH	7.66	7.74	-0.08
5"	C	-	-	-
6"	CH	8.04	7.69	0.36
Mean Absolute Error (MAE) = 0.19 Root Mean Square Error (RMSE) = 0.42				

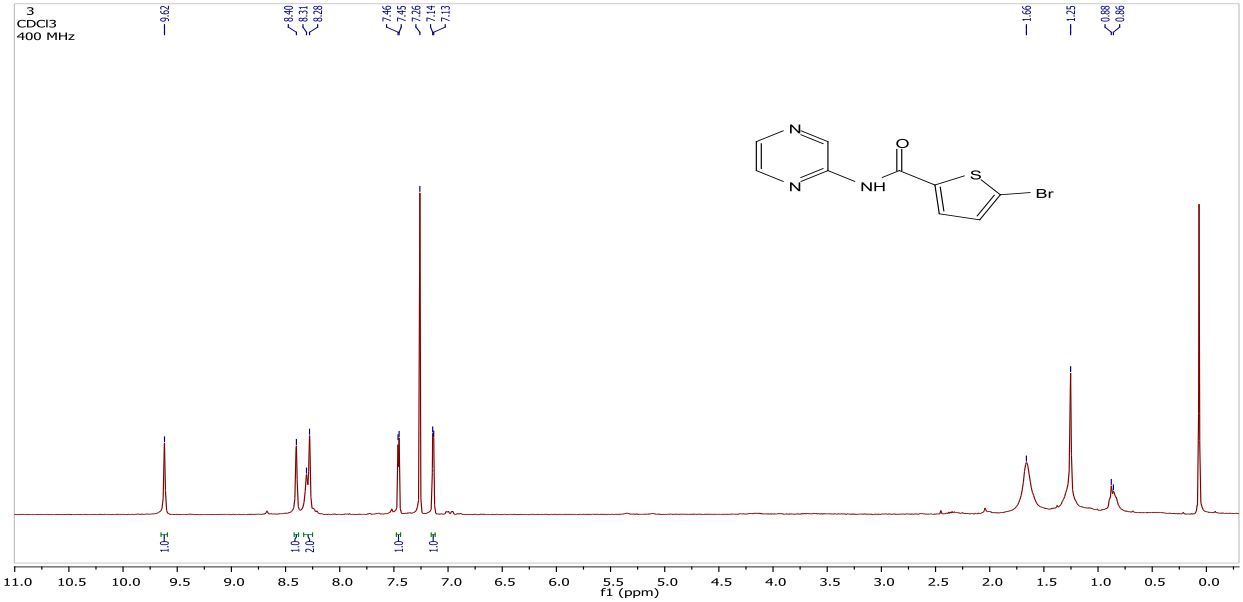

Figure S1: ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3.

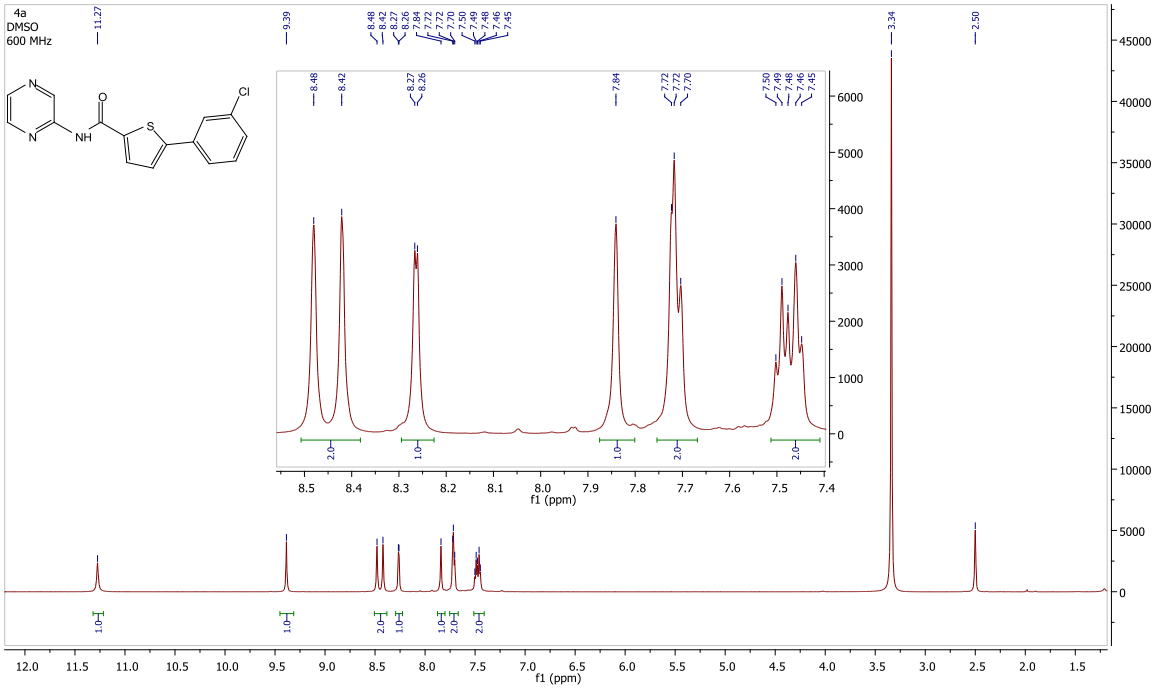

Figure S2: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4a.

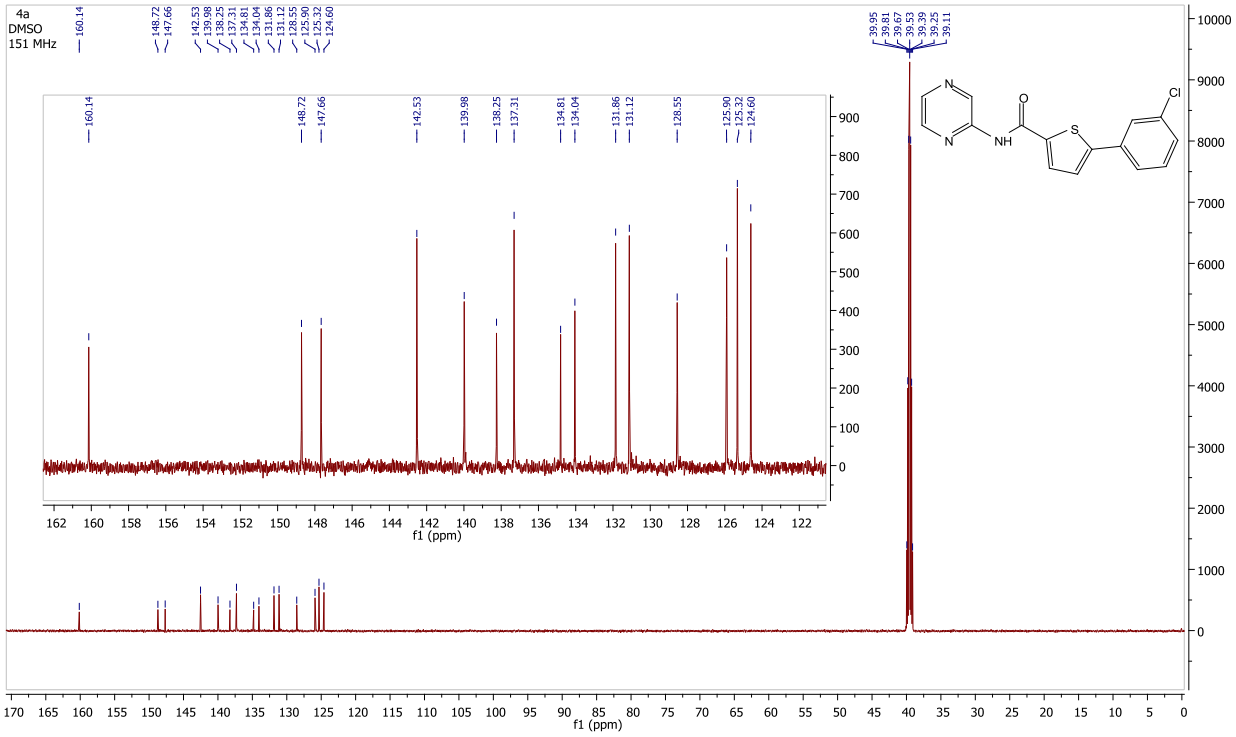

Figure S3: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound 4a.

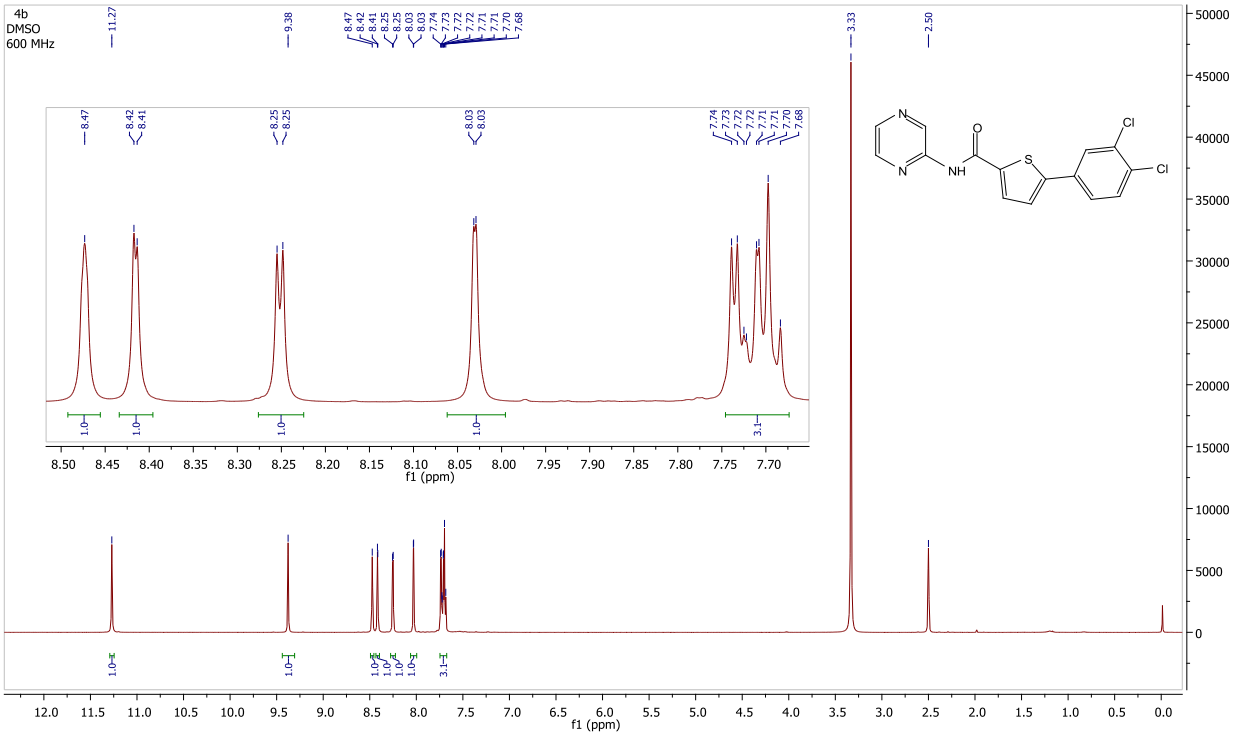

Figure S4: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4b.

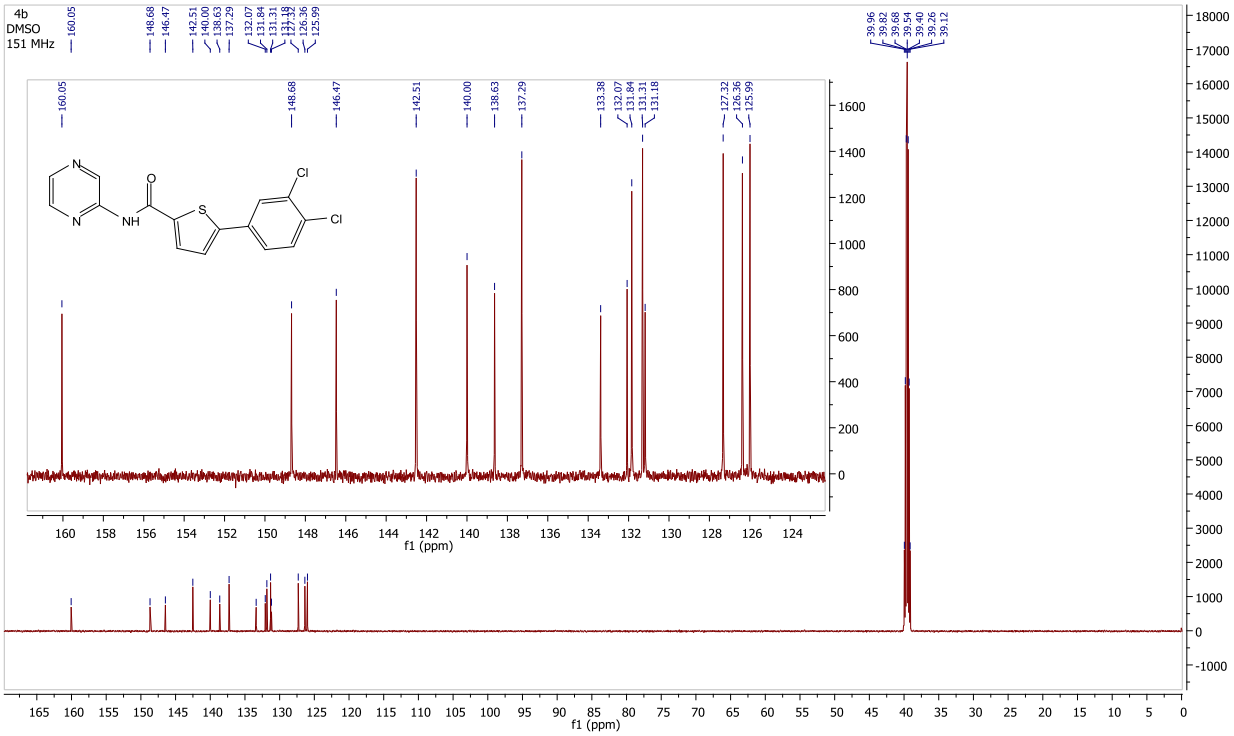

Figure S5: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound 4b.

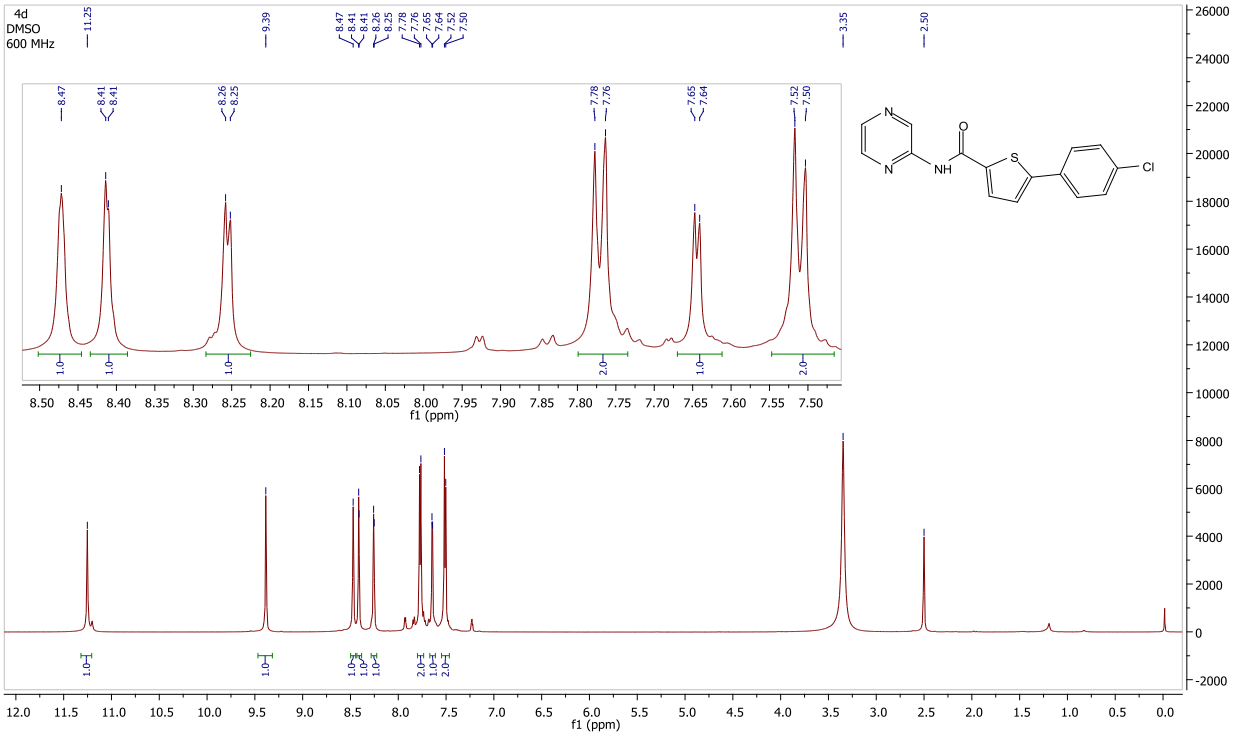

Figure S6: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4d.

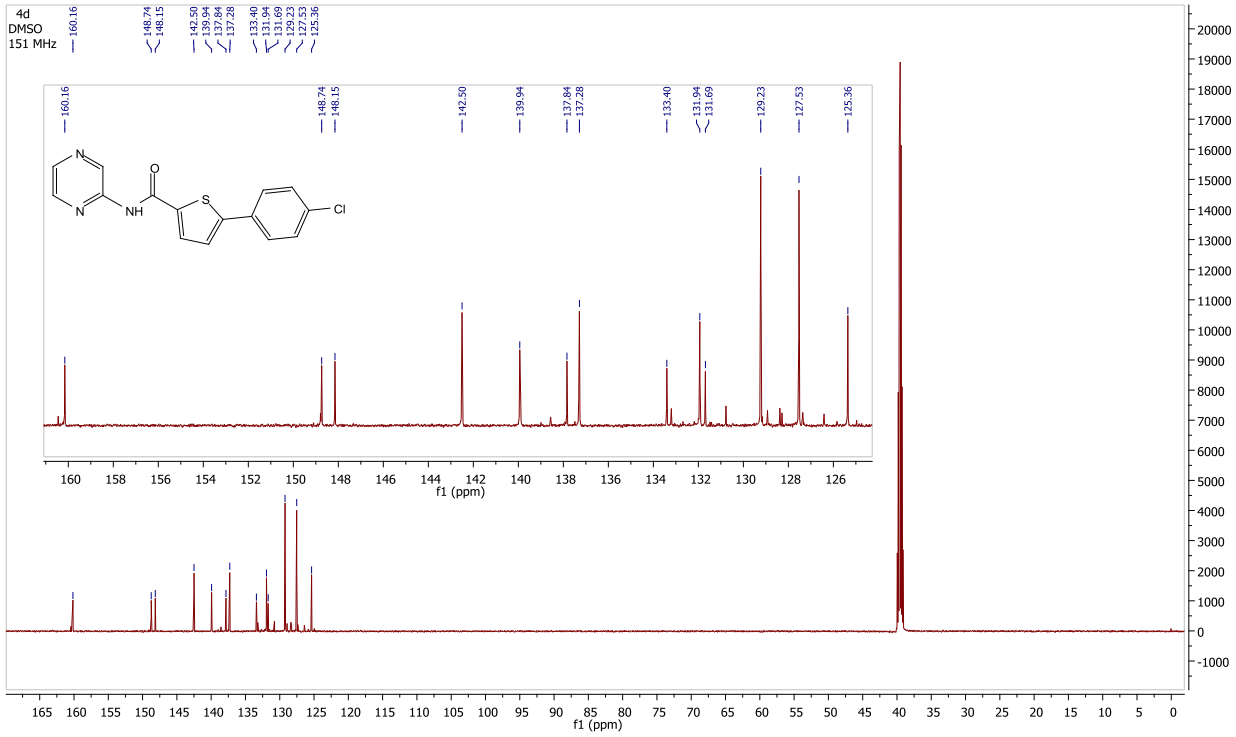

Figure S7: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound 4d.

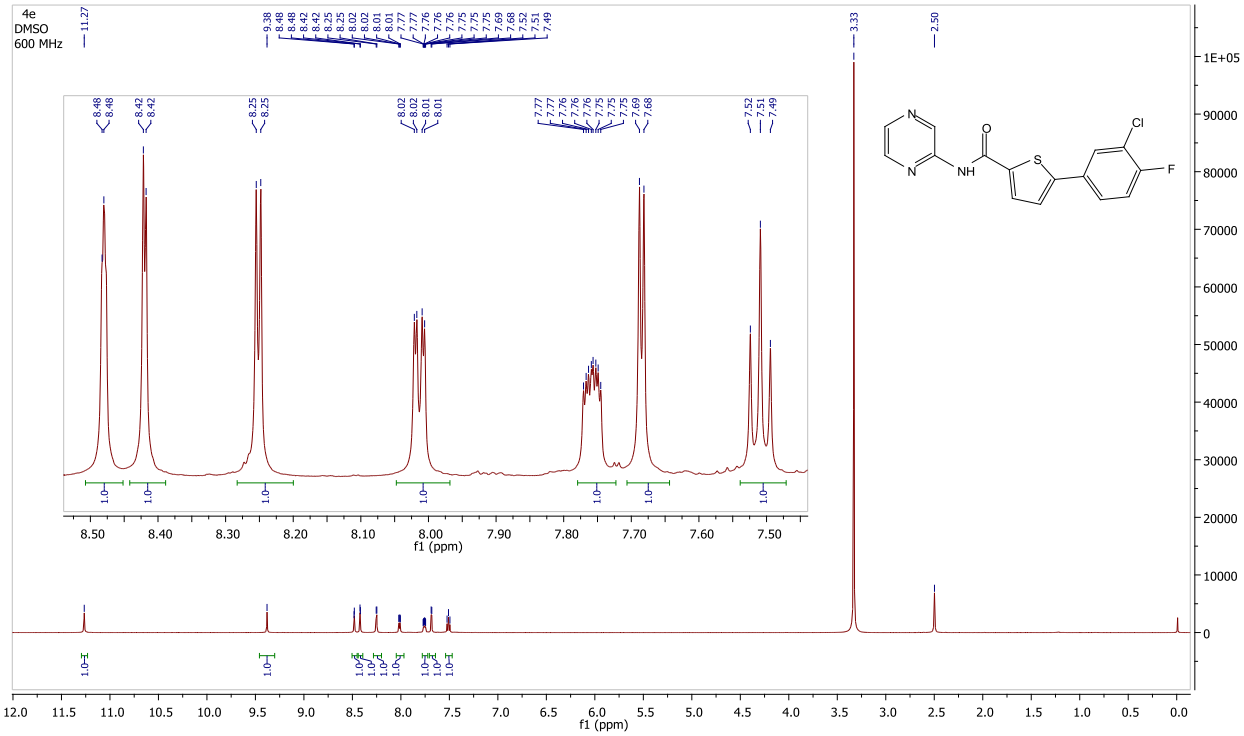

Figure S8: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4e.

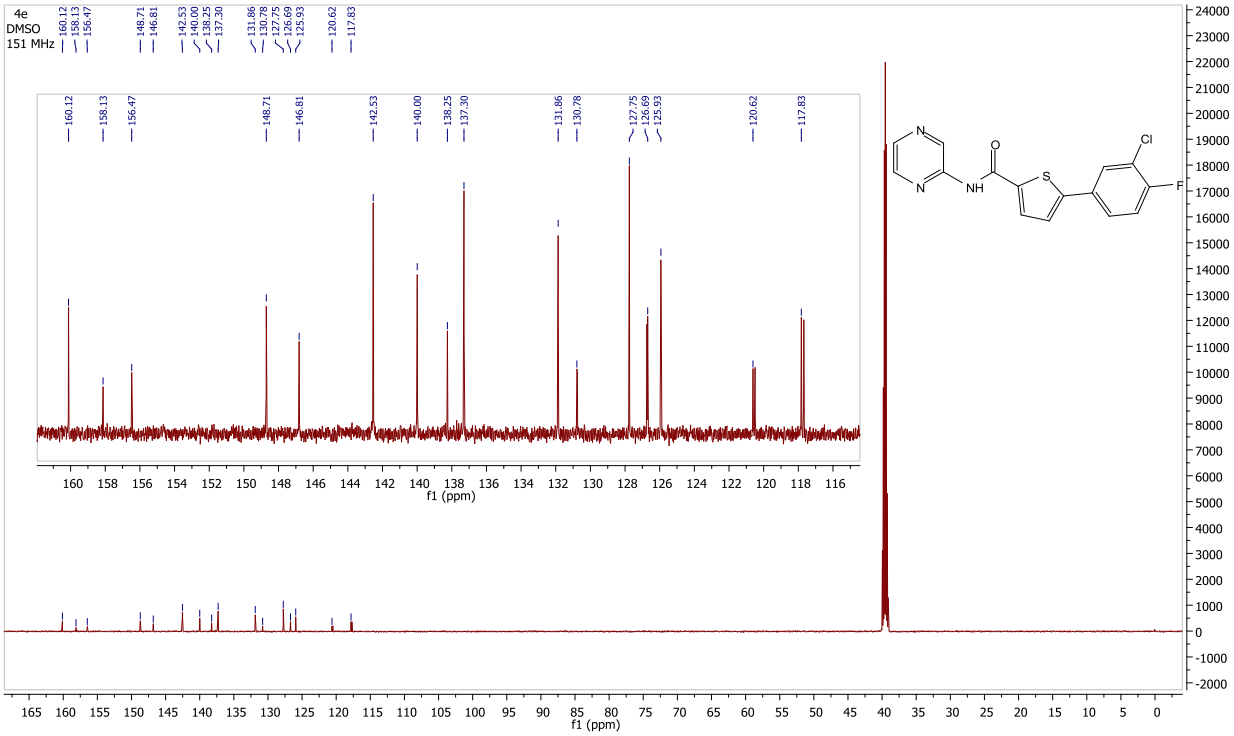

Figure S9: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound 4e.

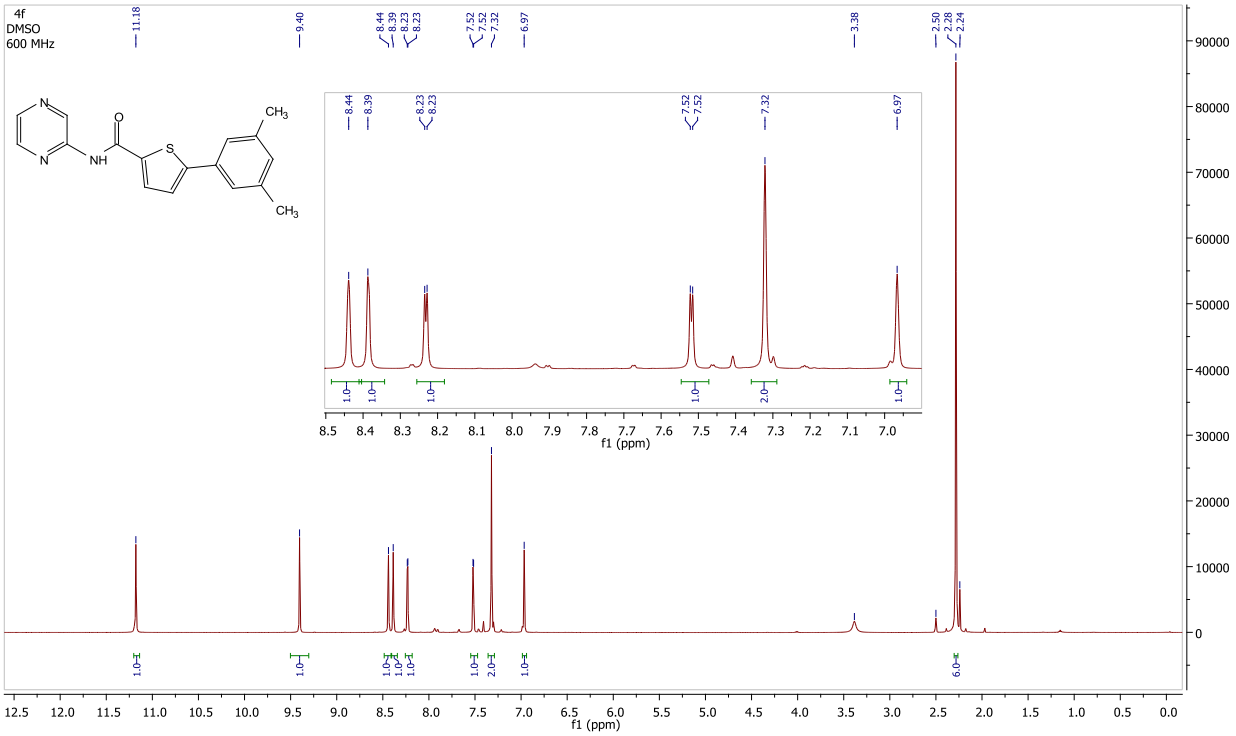

Figure S10: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4f.

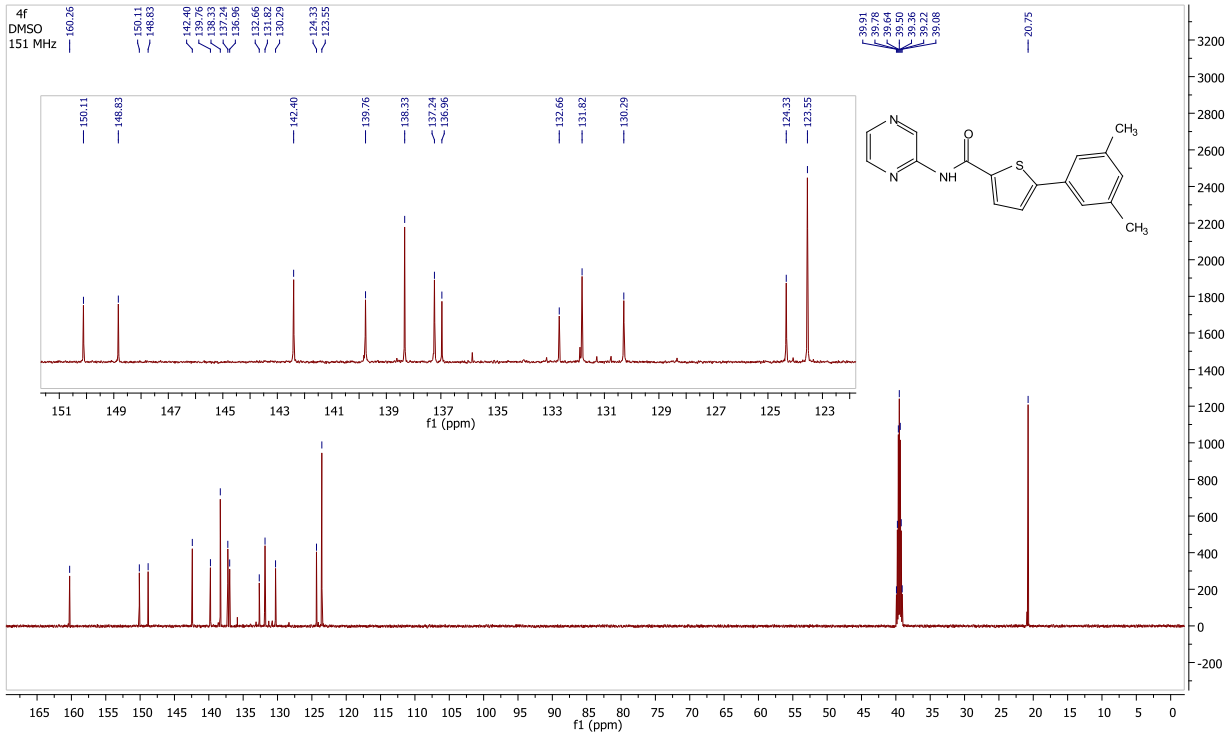

Figure S11: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound 4f.

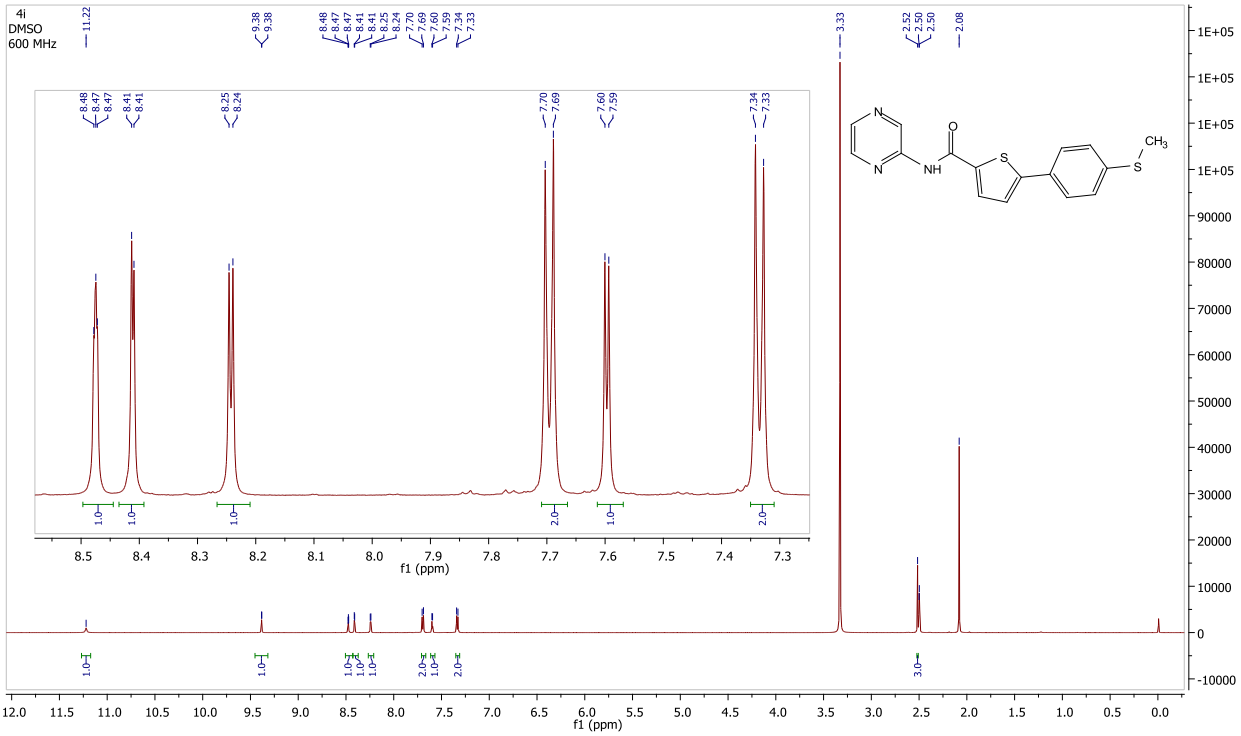

Figure S12: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4i.

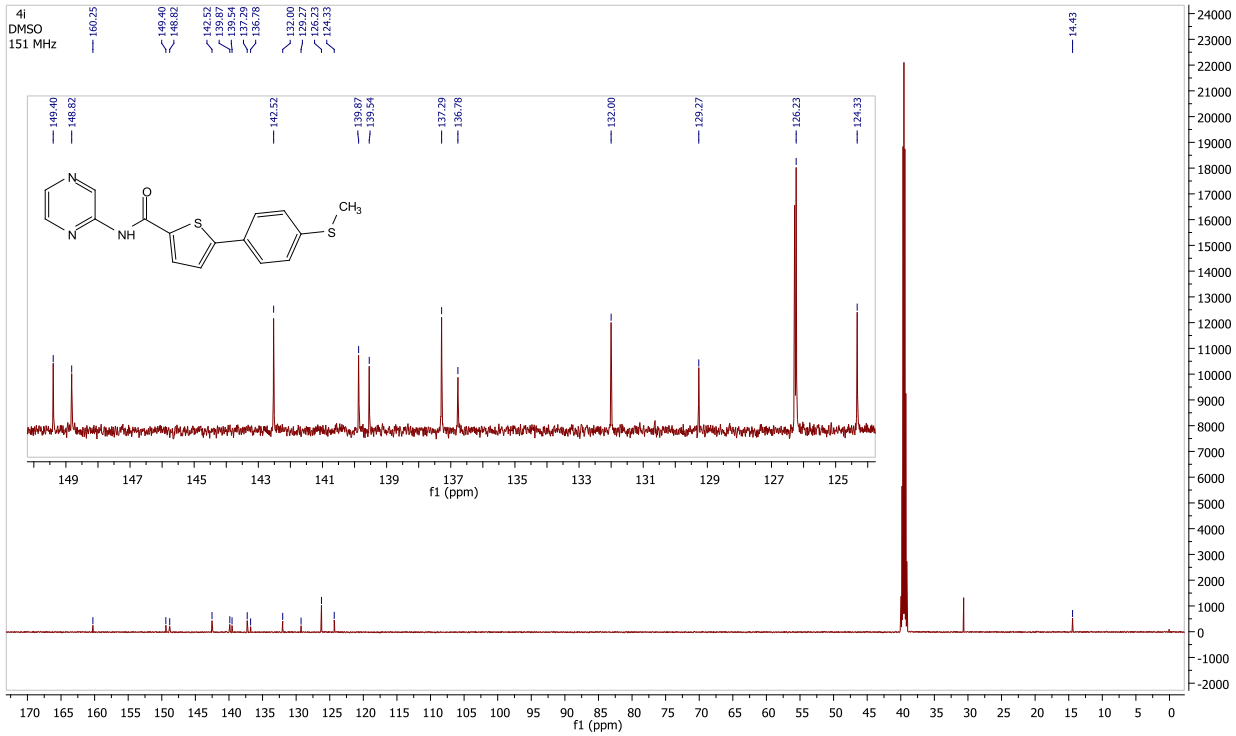

Figure S13: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound 4i.

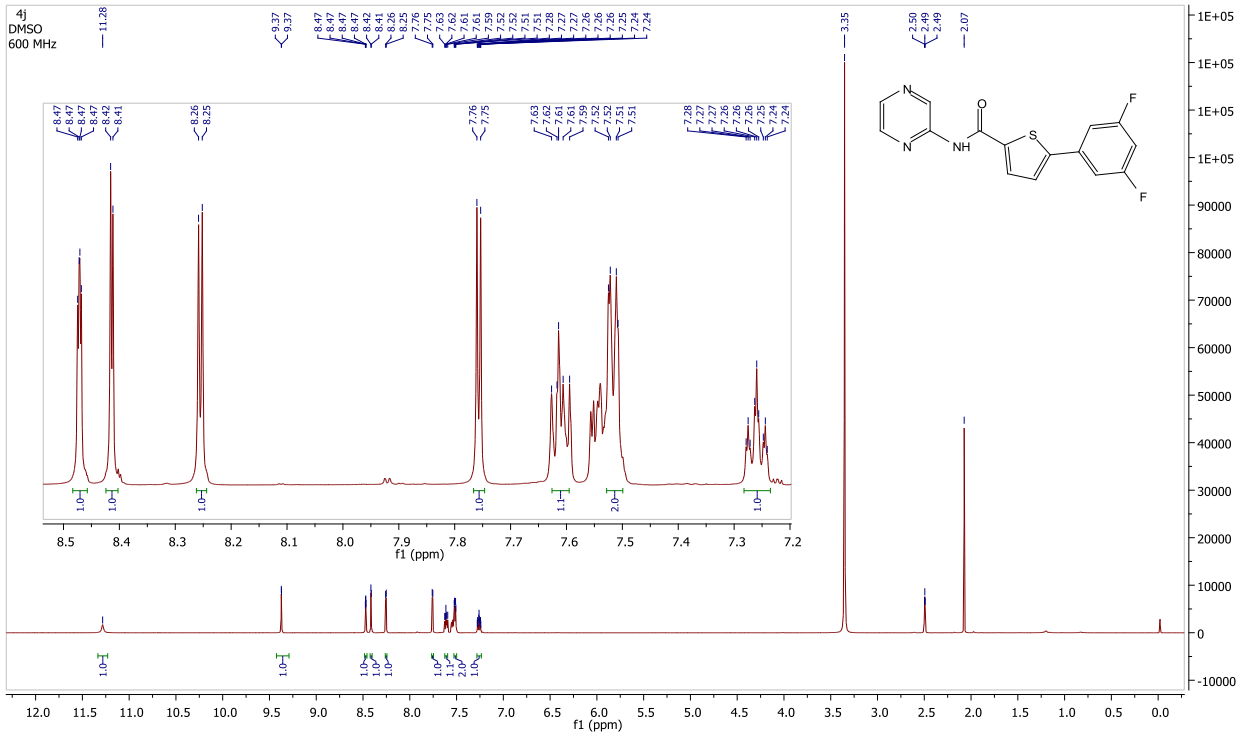

Figure S14: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4j.

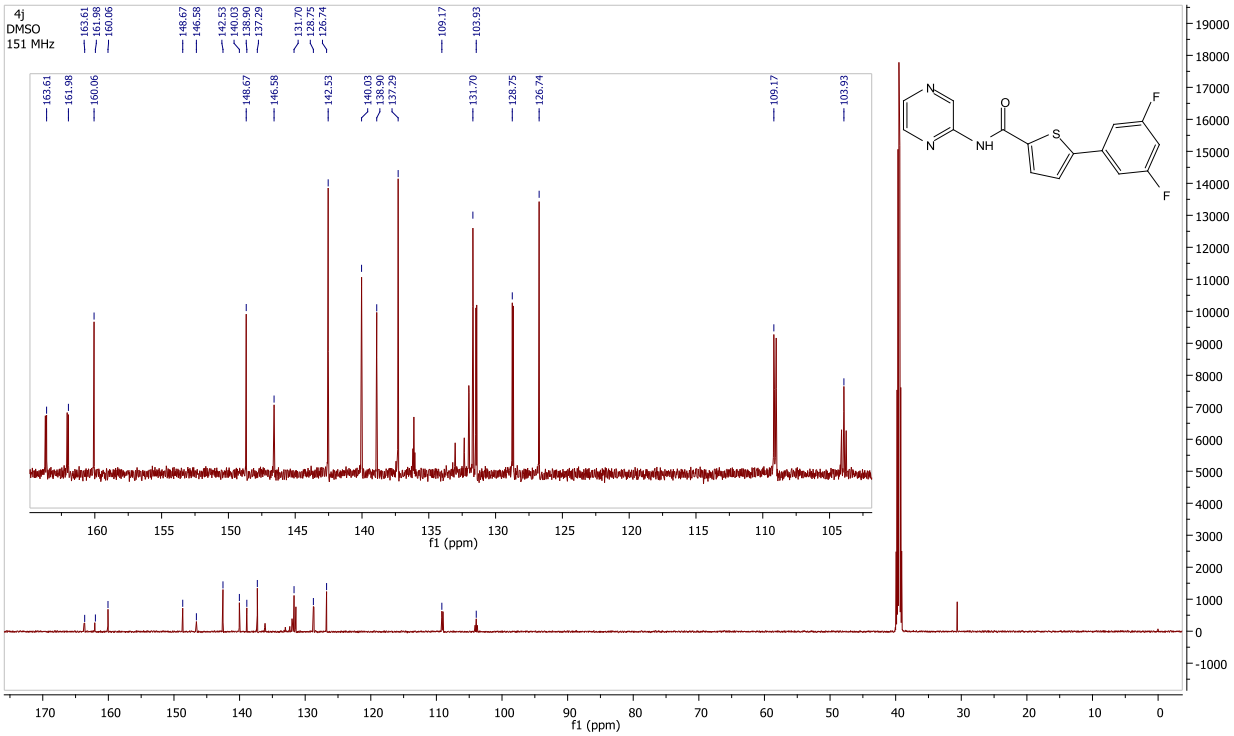

Figure S15: ^{13}C NMR (151 MHz, DMSO-d$_6$) of compound 4j.

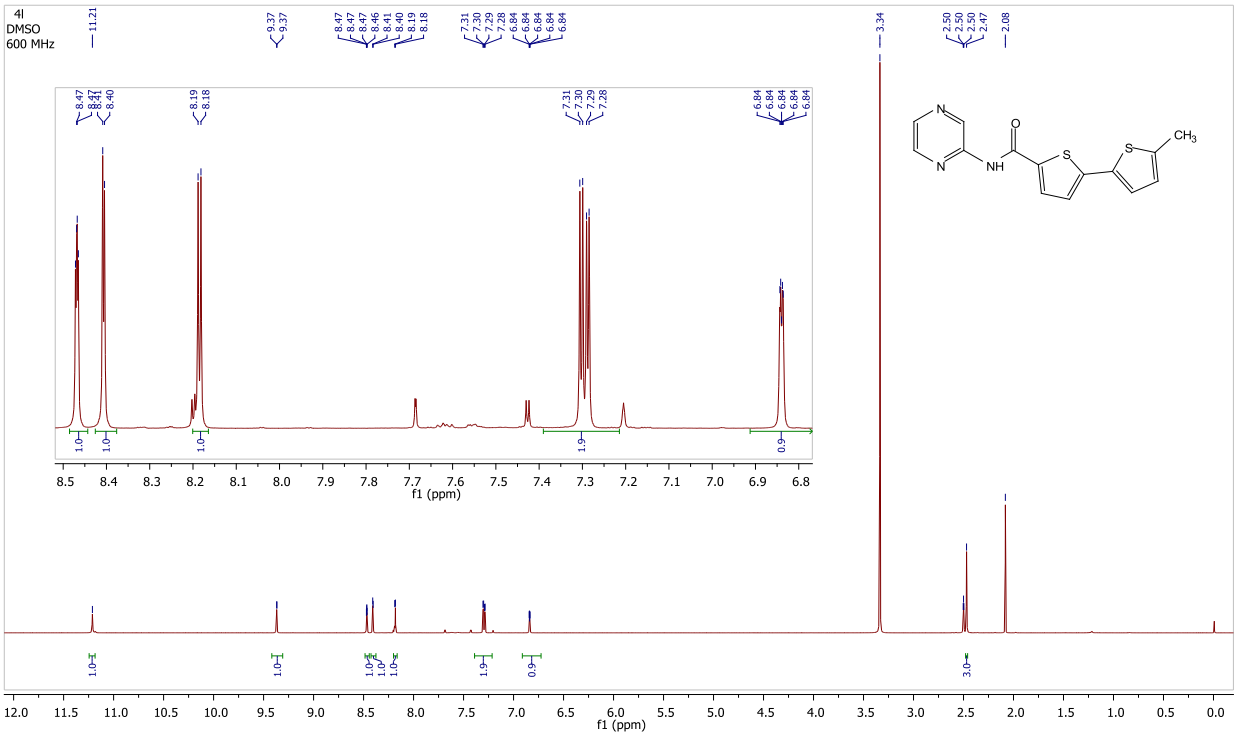

Figure S16: ^{1}H NMR (600 MHz, DMSO-d$_6$) of compound 4l.

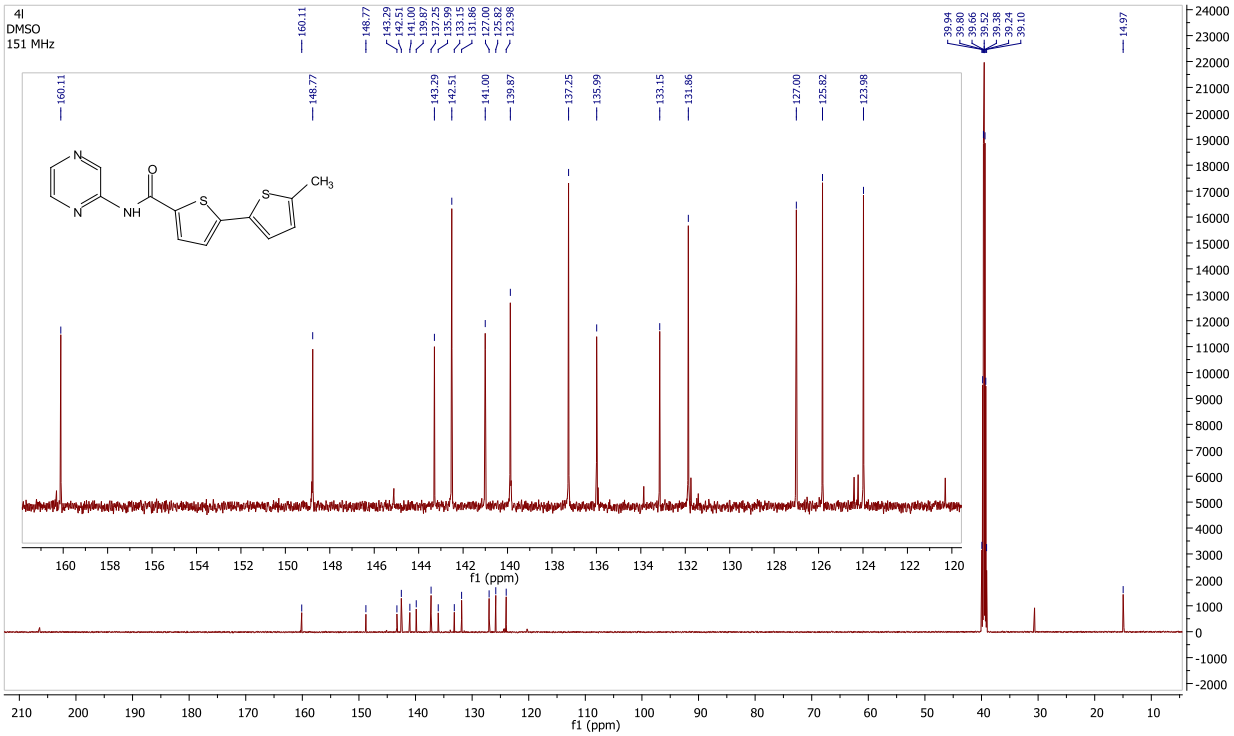

Figure S17: ^{13}C NMR (151 MHz, DMSO-d_6) of compound 4l.

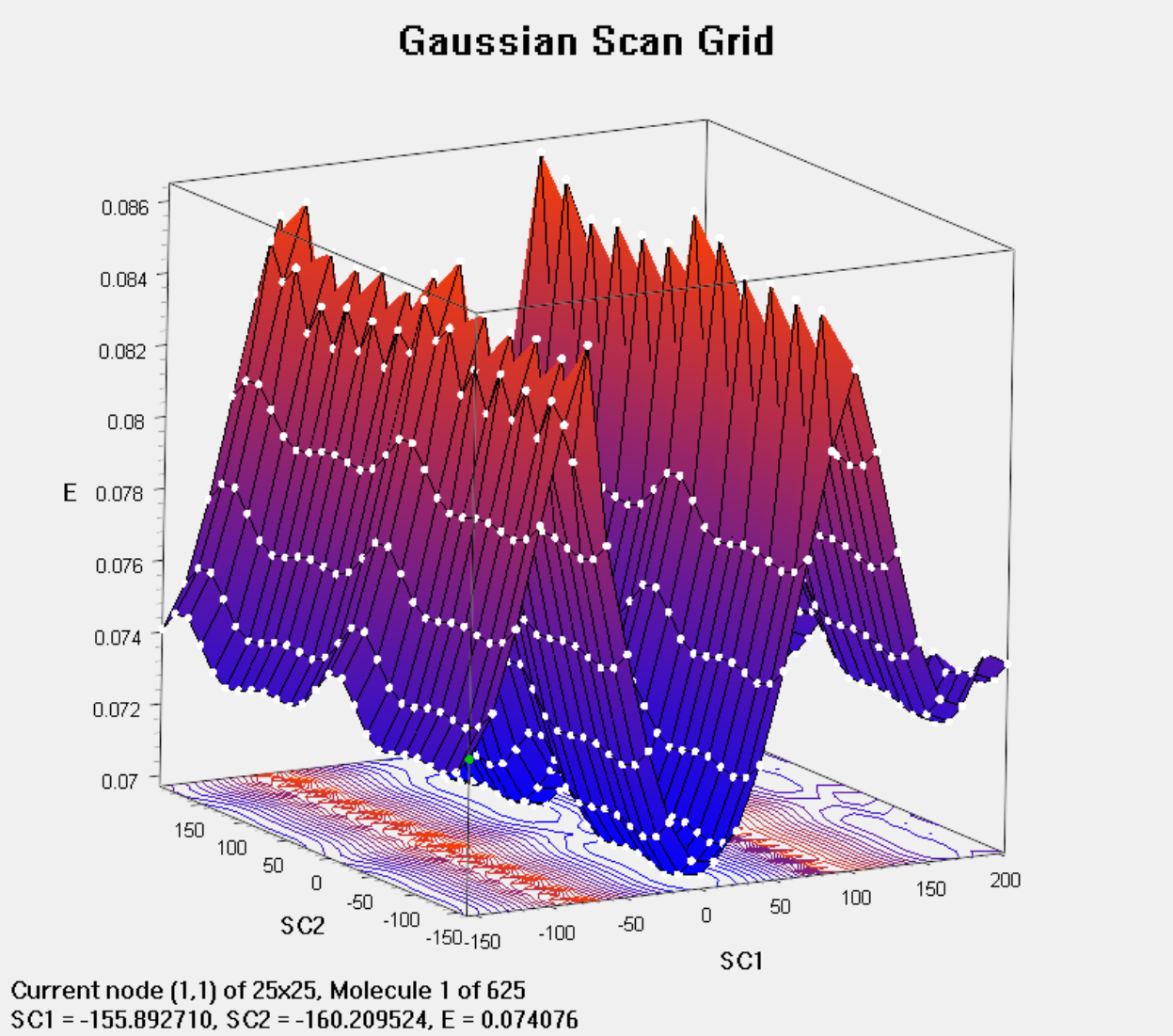

Figure S18. Potential Energy Scan of compound 4a at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

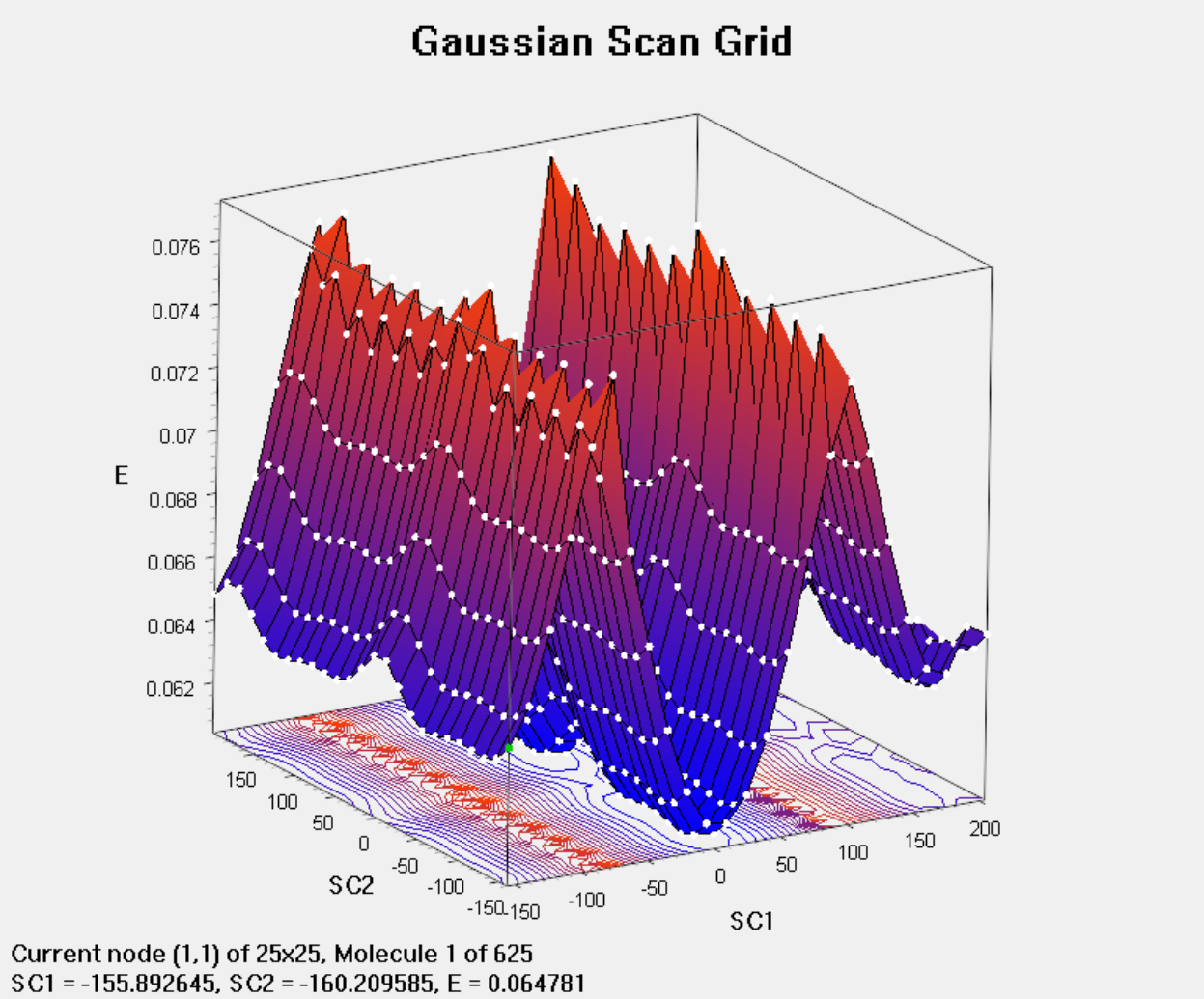

Figure S19. Potential Energy Scan of compound 4b at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

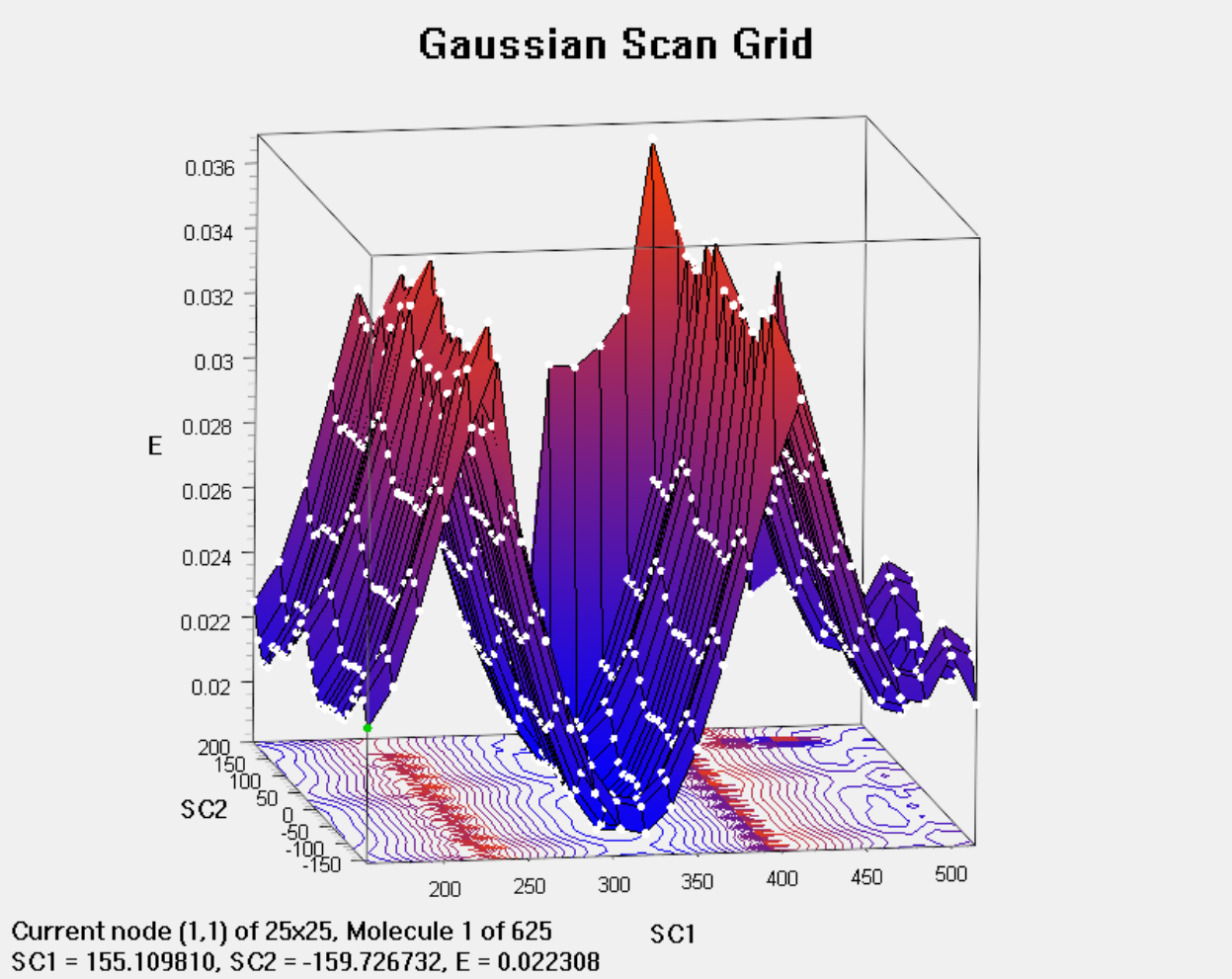

Figure S20. Potential Energy Scan of compound 4c at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

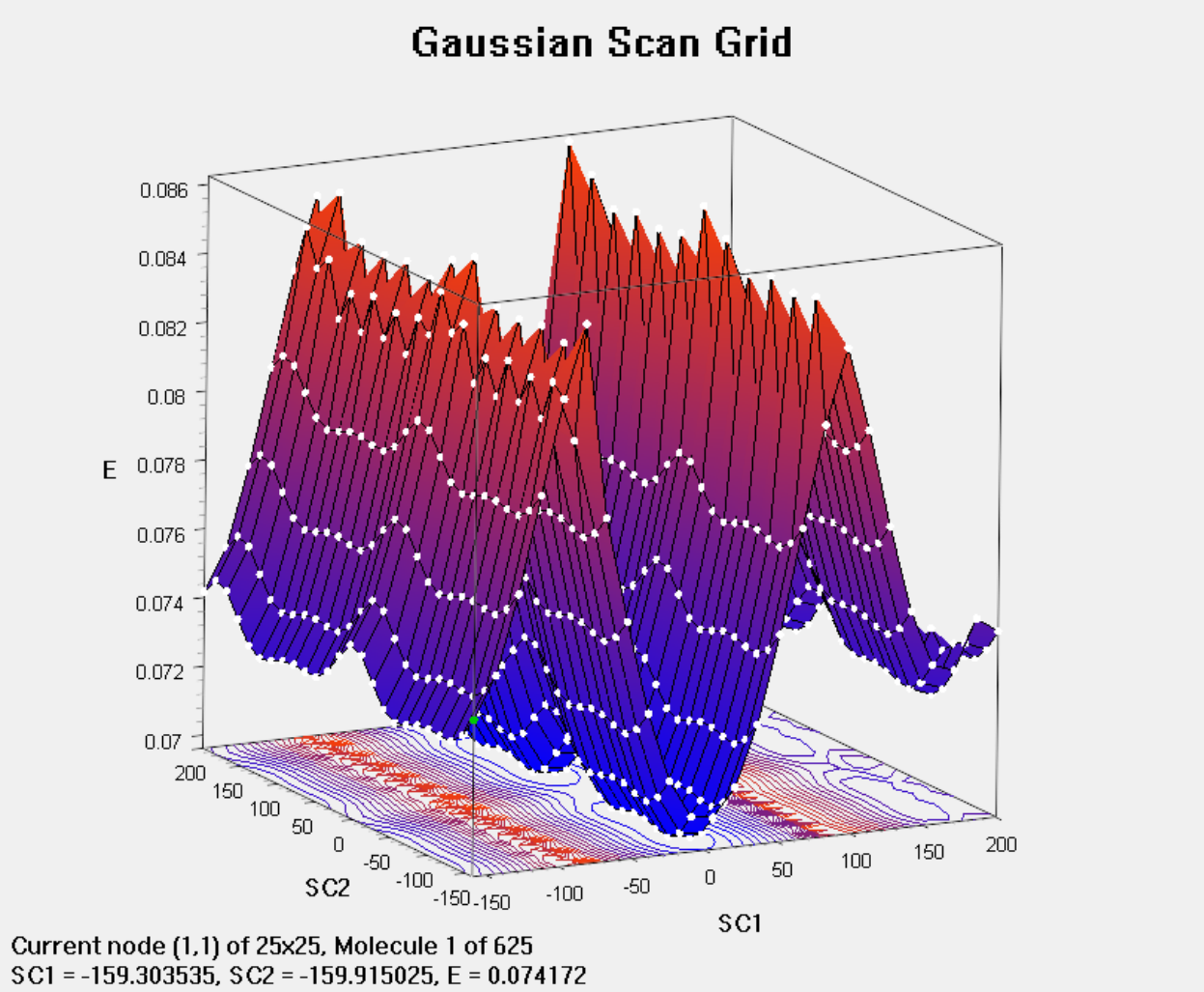

Figure S21. Potential Energy Scan of compound 4d at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

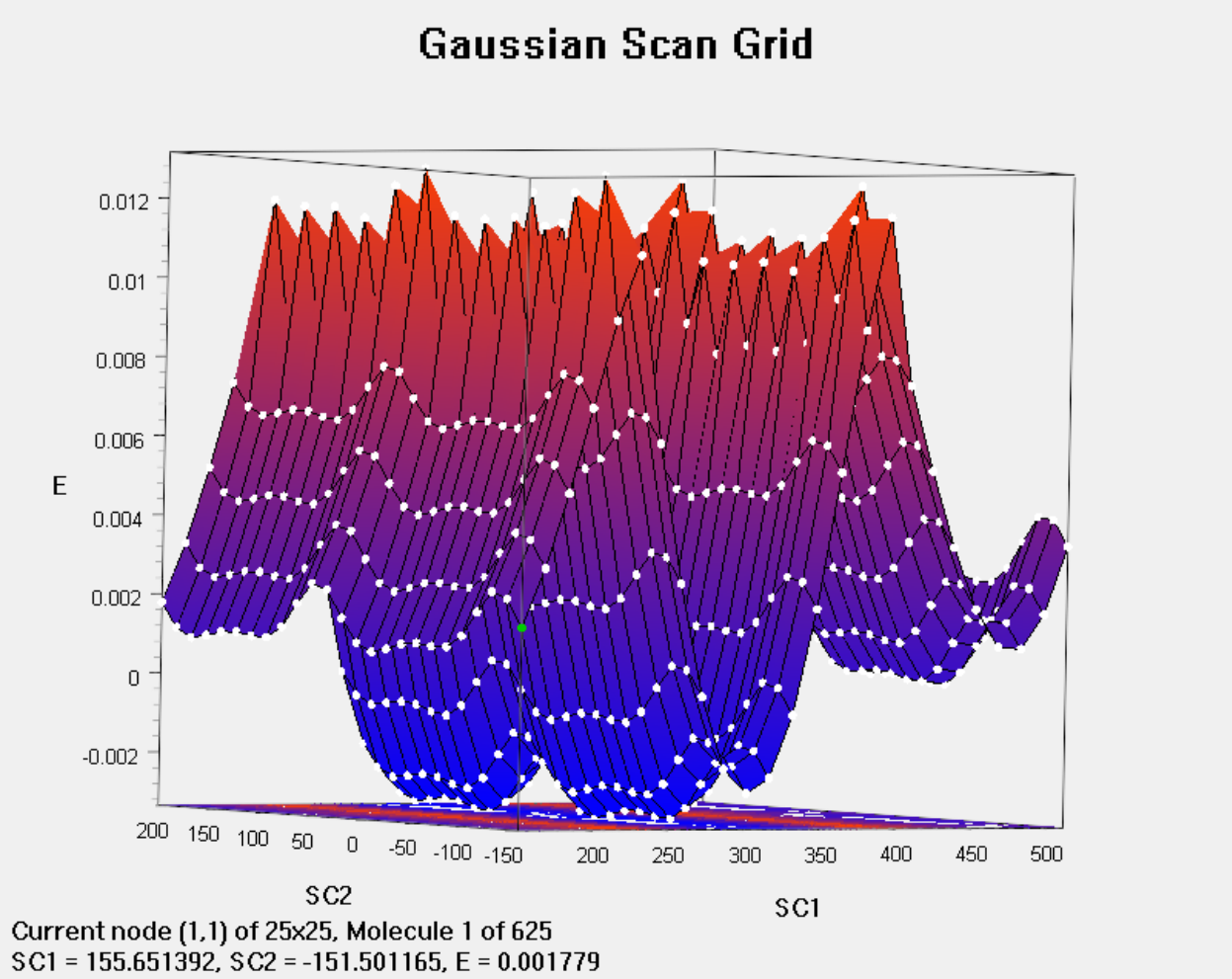

Figure S22. Potential Energy Scan of compound 4e at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

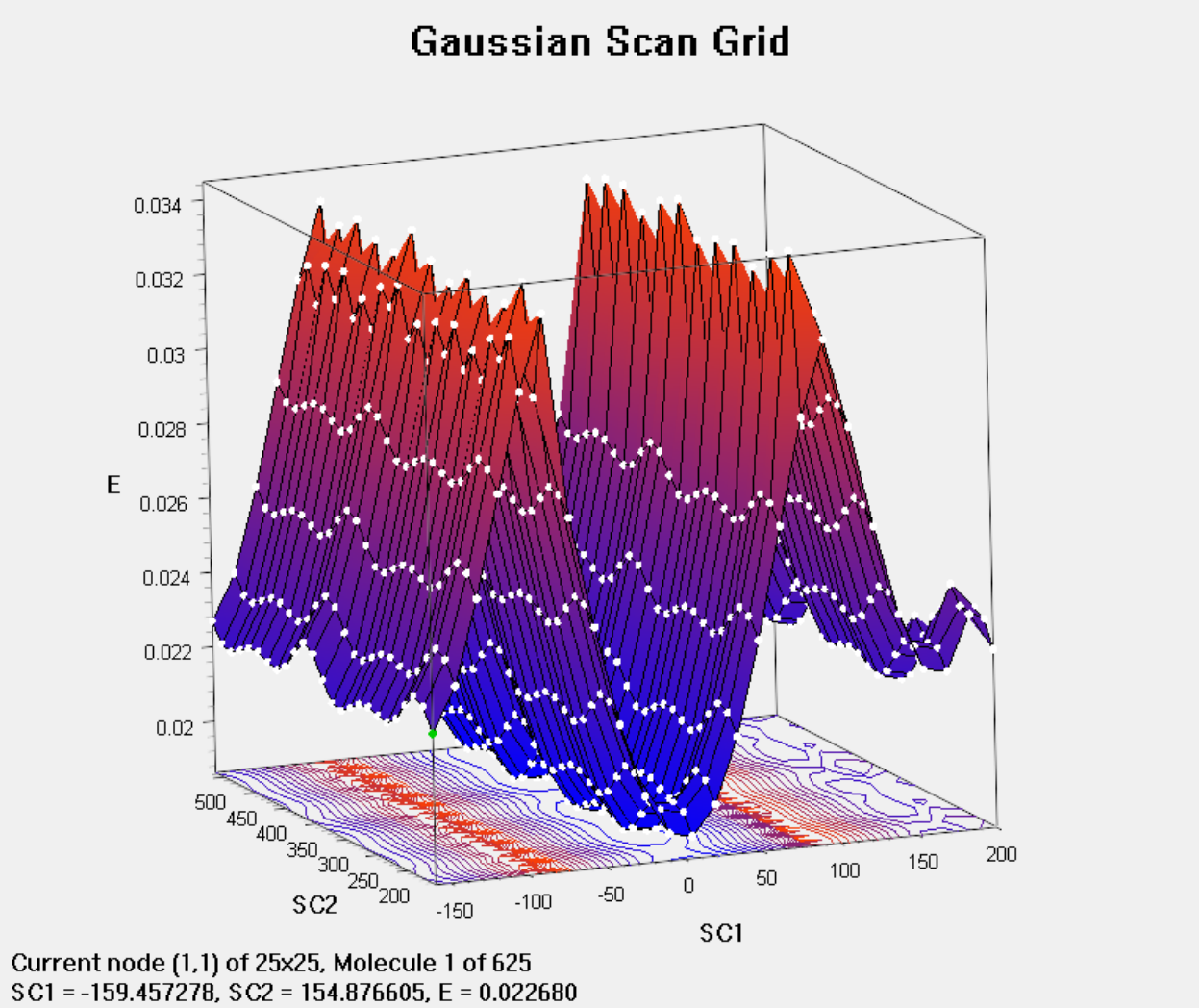

Figure S23. Potential Energy Scan of compound 4g at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

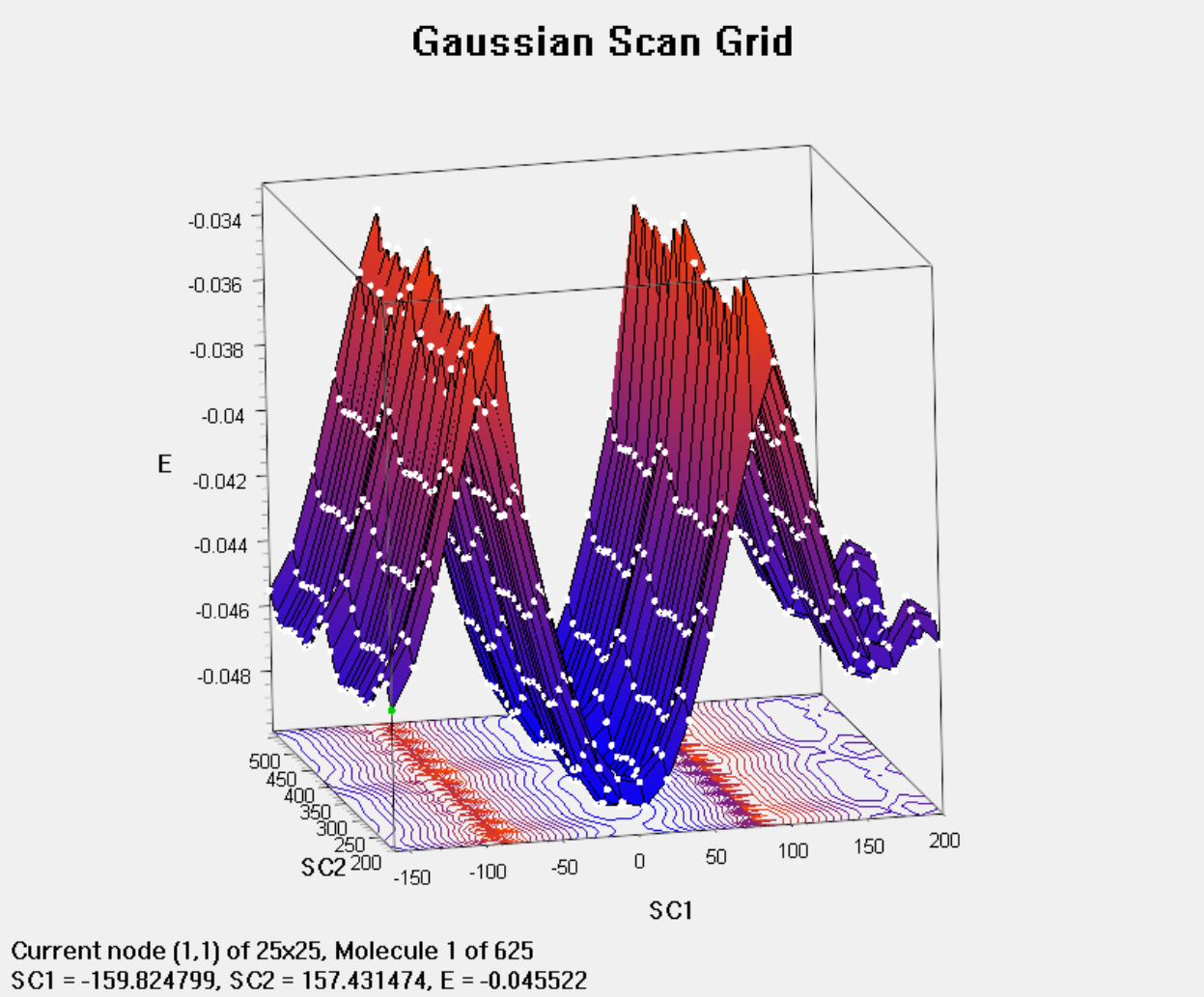

Figure S24. Potential Energy Scan of compound 4h at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

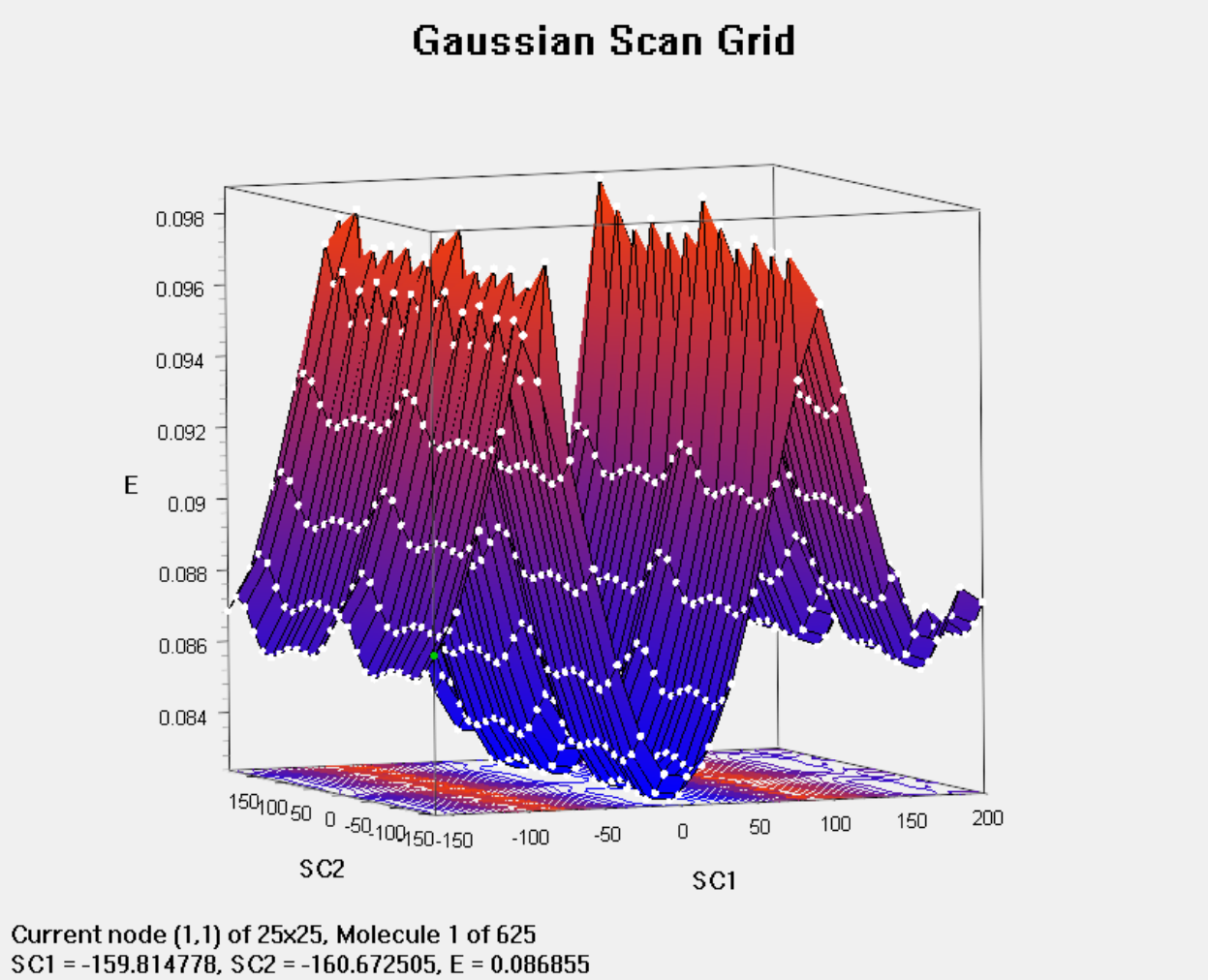

Figure S25. Potential Energy Scan of compound 4i at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

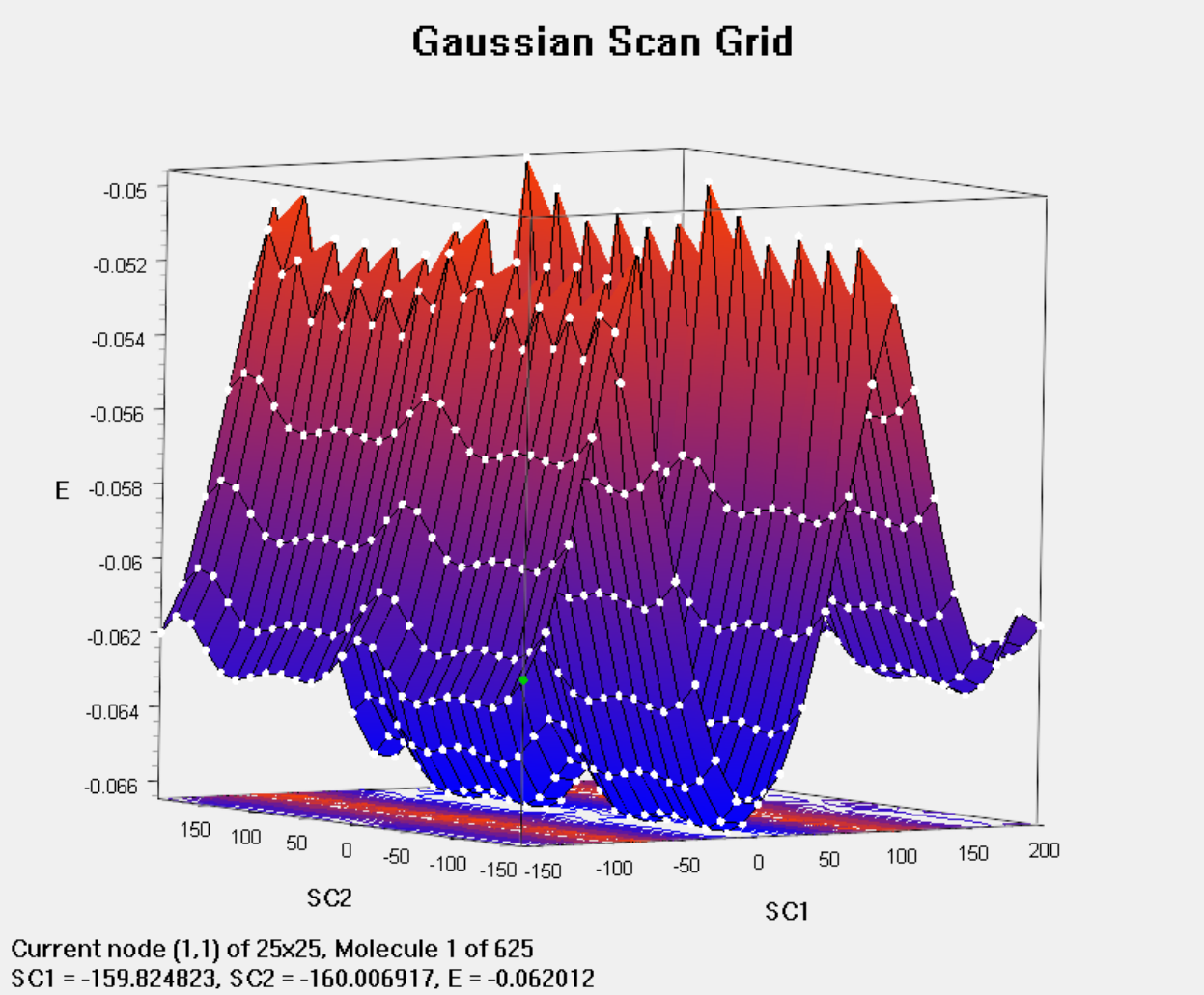

Figure S26. Potential Energy Scan of compound 4j at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

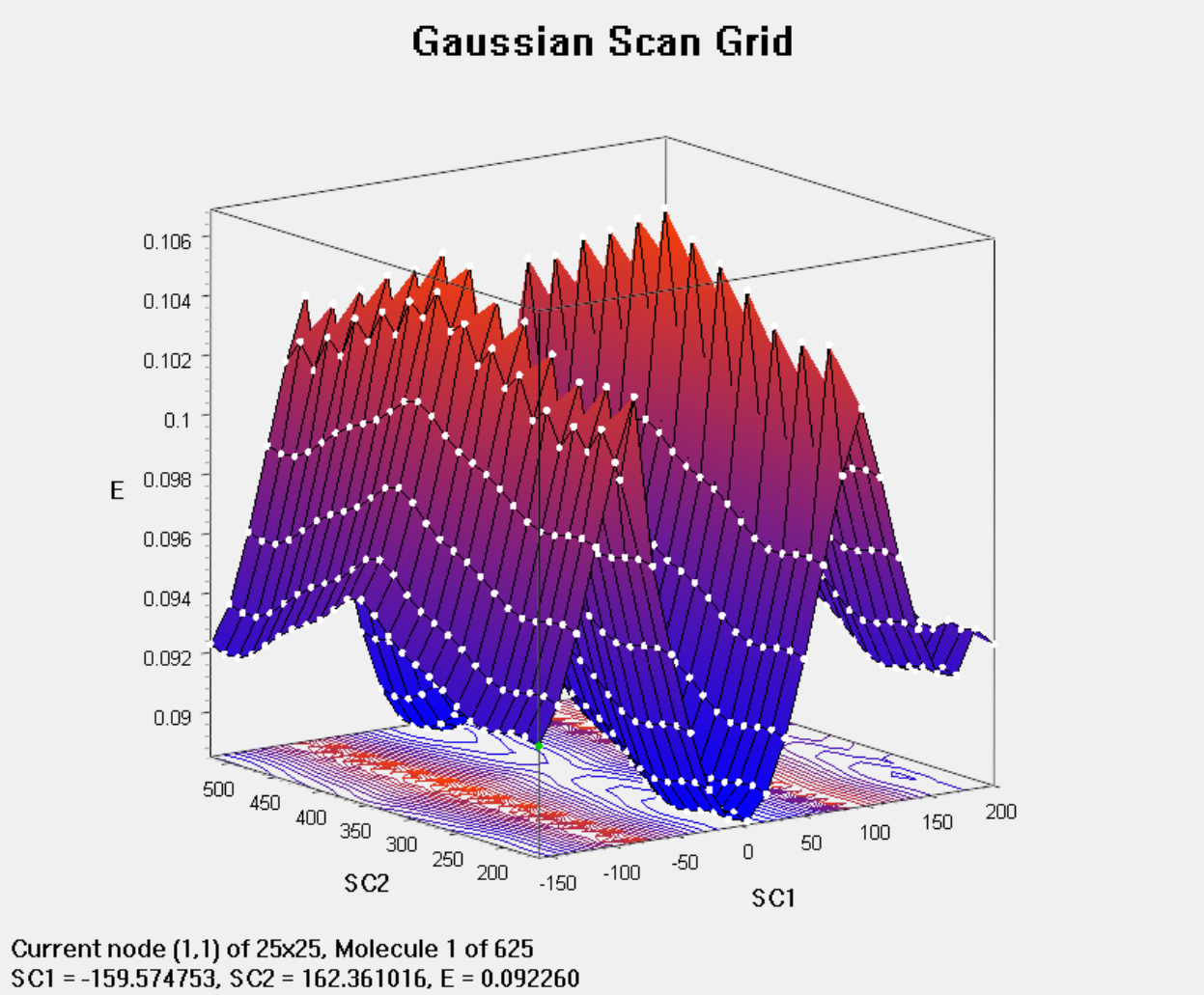

Figure S27. Potential Energy Scan of compound 4k at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

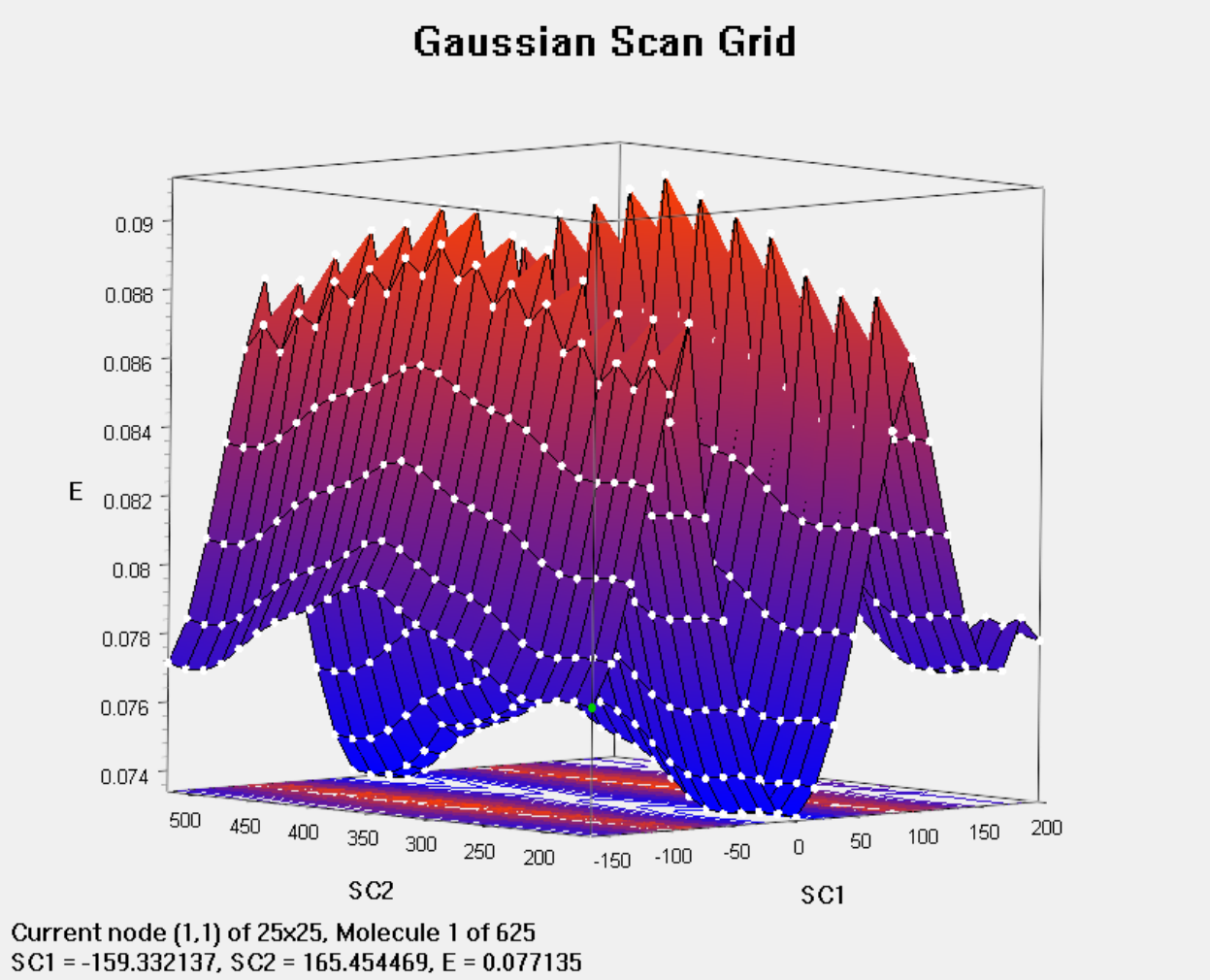

Figure S28. Potential Energy Scan of compound 4l at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

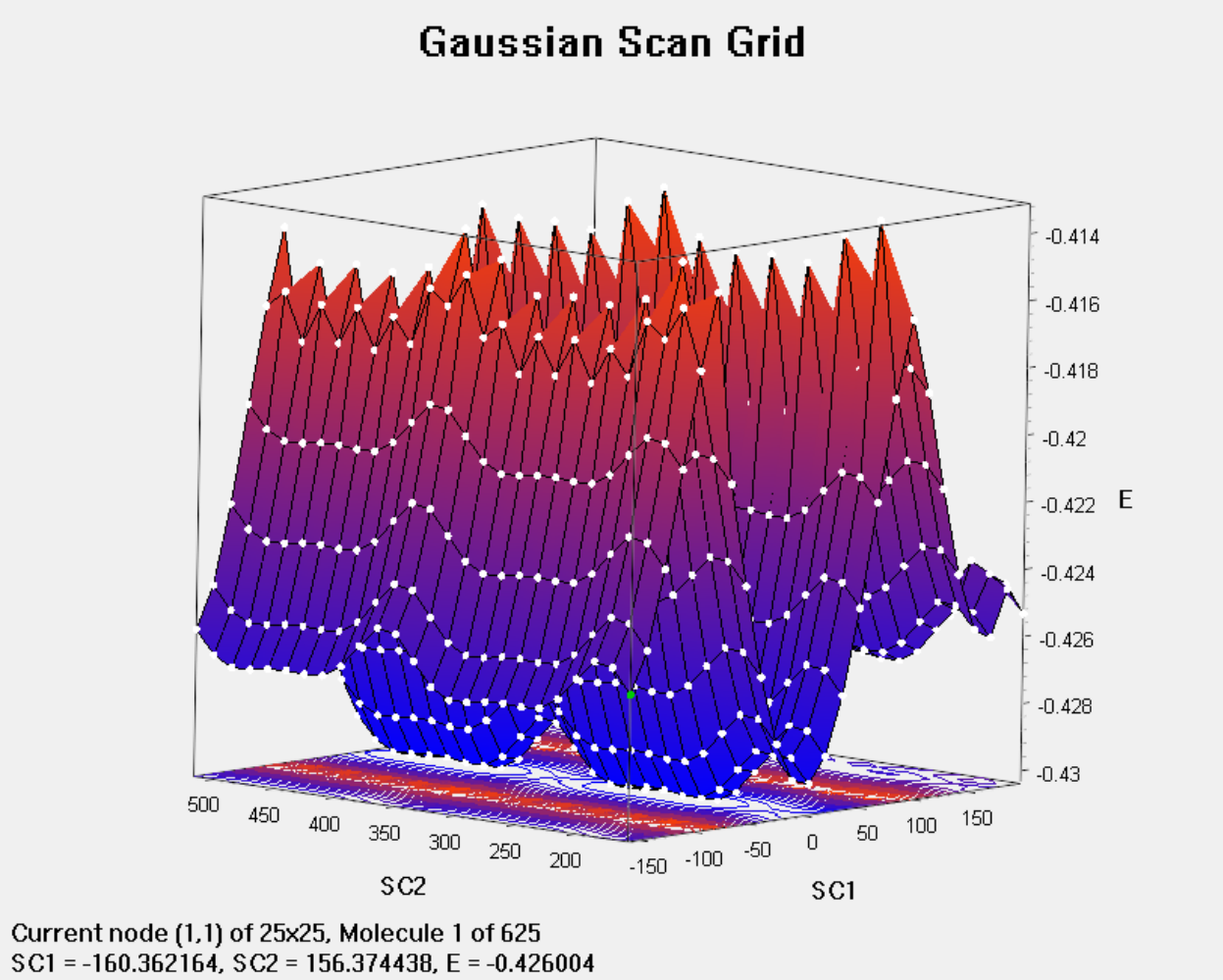

Figure S29. Potential Energy Scan of compound 4m at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

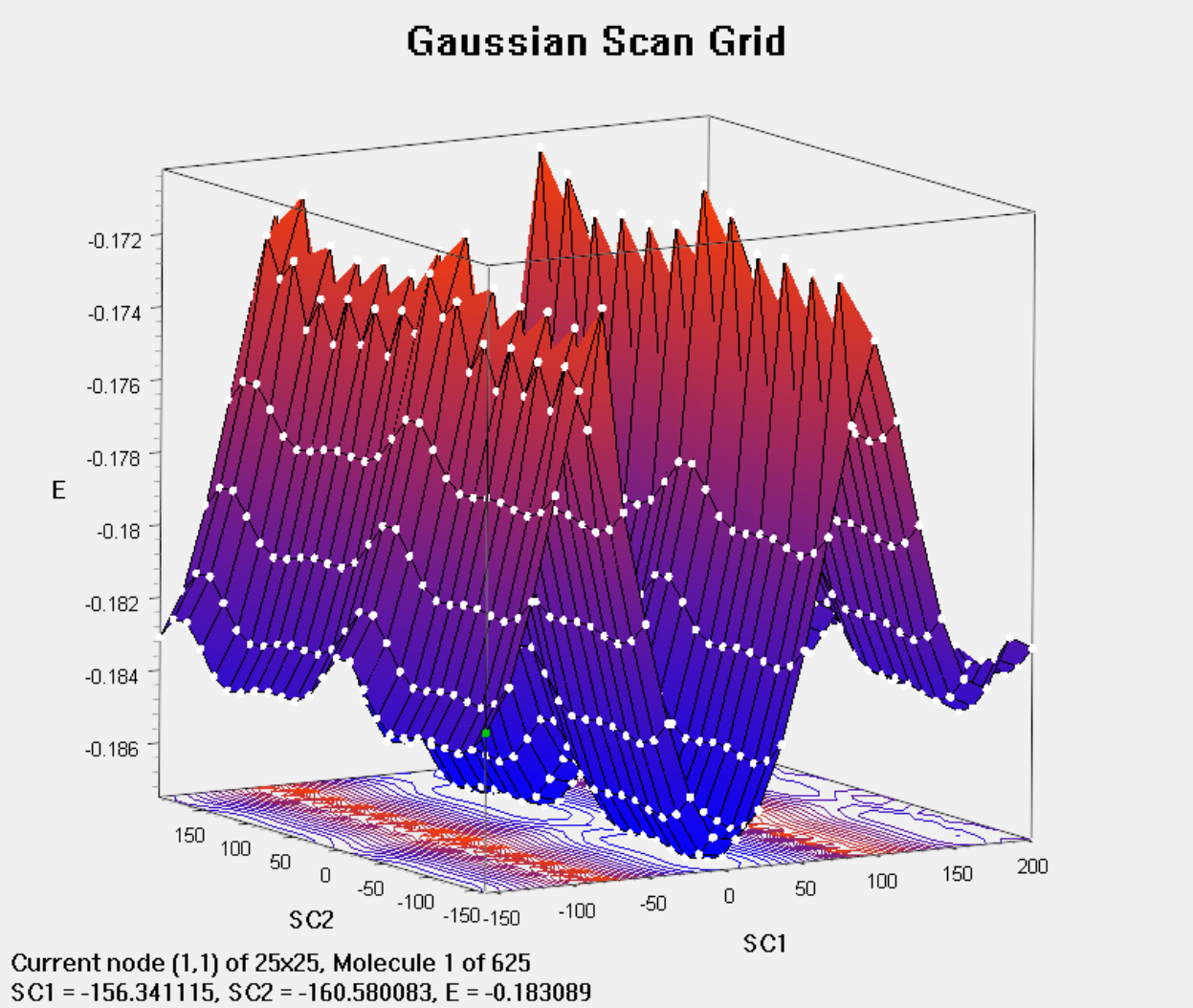

Figure S30. Potential Energy Scan of compound 4n at PBE0-D3BJ/def2-SVP/SMD$_{1,4\text{-dioxane}}$ level of theory

XYZ Coordinates of the lowest energy conformer of 4a

C	-7.28987900	0.01442100	0.31517900
C	-6.78901100	-0.95755400	-0.57535100
N	-5.45757800	-1.10483500	-0.78707600
C	-4.61991300	-0.26745800	-0.09564900
C	-5.13229400	0.71916400	0.80019700
N	-6.45852000	0.84724400	0.99605700
H	-8.36217500	0.13878300	0.49304800
H	-7.44806900	-1.63246900	-1.13320800
H	-4.46285400	1.40339200	1.35071400
N	-3.24068400	-0.48898700	-0.34170700
H	-3.03183600	-1.21801200	-1.03500200
C	-2.19033200	0.29879700	0.19372500
O	-2.40985200	1.27749600	0.88202500
C	-0.83961500	-0.16462100	-0.13169100
C	-0.34996500	-1.35729800	-0.60193200
S	0.44531100	0.95776200	0.15773300
C	1.07597600	-1.35589700	-0.74507300
H	-0.94647400	-2.22962000	-0.84026200
C	1.65260700	-0.16348700	-0.38201900
H	1.62218500	-2.21524800	-1.11295300
C	3.05666100	0.22262000	-0.38216500
C	4.00207600	-0.60673100	0.24690300
C	3.47107500	1.41368100	-1.00321000
C	5.34142400	-0.21802500	0.23900600
H	3.69136700	-1.52992400	0.73698100
C	4.82102100	1.77660300	-0.99440400
H	2.74325500	2.05433100	-1.50194600
C	5.77160400	0.96299200	-0.37130800
H	6.82495500	1.24258400	-0.36114400
H	5.13608100	2.70207100	-1.47806600
Cl	6.50566300	-1.23160300	1.00927900

XYZ Coordinates of the lowest energy conformer of 4b

C	-7.93083700	-0.05475000	-0.45525000
C	-7.40251400	1.20925700	-0.11988200
N	-6.07344400	1.39092500	0.07854400
C	-5.26613300	0.29112400	-0.06150500
C	-5.80520800	-0.98555900	-0.40360400
N	-7.12907100	-1.14347400	-0.59524600
H	-9.00184200	-0.21017600	-0.61636200
H	-8.03744300	2.09527300	-0.00556500
H	-5.15916700	-1.87327500	-0.52258700
N	-3.88962200	0.54604300	0.16871000
H	-3.65503500	1.52252800	0.38597900
C	-2.86150200	-0.42240200	0.06220500
O	-3.08879300	-1.56640700	-0.28305900
C	-1.51785600	0.06327200	0.38994100
C	-1.06744800	1.12599300	1.13157700
S	-0.19465200	-0.87654100	-0.20878500
C	0.36292200	1.18686900	1.20513000
H	-1.69608000	1.85227700	1.63265900
C	0.98070700	0.16601800	0.52549800
H	0.88172800	1.96026100	1.75742200
C	2.40014700	-0.10767500	0.35844200
C	3.25408200	0.91649600	-0.08838400
C	2.91977000	-1.38462500	0.63864200
C	4.61376400	0.64905300	-0.25106300
H	2.85730600	1.90851100	-0.31272600
C	4.28166600	-1.64387800	0.47332700
H	2.26178600	-2.17875800	0.99691600
C	5.12757700	-0.62437600	0.02719500
H	4.68572900	-2.63463400	0.69108600
Cl	5.66063100	1.89041300	-0.79578500
Cl	6.79807000	-0.93449900	-0.17830100

XYZ Coordinates of the lowest energy conformer of 4c

C	-7.37184300	0.78869800	-0.06218700
C	-7.03238100	-0.36360700	0.67660600
N	-5.74512400	-0.77230100	0.79918000
C	-4.78834800	-0.01571200	0.17209200
C	-5.13677200	1.15178300	-0.57202700
N	-6.42203100	1.53913200	-0.68096000
H	-8.40771800	1.12490200	-0.16678300
H	-7.78776700	-0.97621600	1.18181100
H	-4.36962300	1.76764400	-1.07395600
N	-3.46569200	-0.50398100	0.32771800
H	-3.37687700	-1.34987400	0.90343600
C	-2.30731500	0.12792000	-0.18807400
O	-2.36970700	1.17695300	-0.80265300
C	-1.04558600	-0.57237100	0.05773100
C	-0.72950800	-1.77252100	0.64247500
S	0.38204800	0.23450300	-0.50093300
C	0.67905700	-2.03742800	0.64756400
H	-1.44080600	-2.47156000	1.06526900
C	1.41868100	-1.03641000	0.06761200
H	1.09660000	-2.93656700	1.08206800
C	2.85740700	-0.93368500	-0.12072700
C	3.56832100	-2.00932300	-0.68495800
C	3.54169500	0.23336000	0.25762800
C	4.94914700	-1.91619700	-0.86491700
H	3.03642500	-2.91270200	-0.98518500
C	4.92510600	0.32244500	0.06993200
H	2.99427500	1.06068100	0.71151600
C	5.62991900	-0.75639400	-0.48448300
H	5.49913100	-2.75092300	-1.29958200
H	6.71432400	-0.68368200	-0.60831000
C	5.70009800	1.54673600	0.46575700
O	6.86247300	1.46701700	0.79799600
C	4.98081100	2.86182400	0.40691800
H	4.39148800	2.97987400	-0.51136400
H	4.30024100	2.98961700	1.26003700
H	5.69441300	3.70035100	0.45001700

XYZ Coordinates of the lowest energy conformer of 4d

C	-7.38336100	-0.41920600	0.01334300
C	-6.92486000	0.79754000	0.55908800
N	-5.60253100	1.09247900	0.62045400
C	-4.73111700	0.15526200	0.12722300
C	-5.20015200	-1.07779100	-0.41891100
N	-6.51811800	-1.34940100	-0.47094400
H	-8.44816000	-0.66432800	-0.04145200
H	-7.61111100	1.55413600	0.95616600
H	-4.50231600	-1.84043900	-0.80723900
N	-3.36608500	0.53357300	0.19823300
H	-3.18631400	1.44098900	0.64554000
C	-2.27916800	-0.29508900	-0.18046600
O	-2.44670500	-1.43968500	-0.55619300
C	-0.96107600	0.33736300	-0.09478500
C	-0.55855900	1.64810100	-0.04340800
S	0.40438000	-0.72635800	-0.10689700
C	0.86665800	1.79189400	0.00542300
H	-1.21891900	2.50689400	-0.04757300
C	1.53056000	0.59012300	-0.01019600
H	1.34946500	2.75907800	0.05937800
C	2.96012900	0.32114100	0.02177900
C	3.50007500	-0.55098000	0.98390400
C	3.80557500	0.93978000	-0.91814400
C	4.87254000	-0.80662500	1.00785000
H	2.85122200	-1.02549900	1.72174900
C	5.17808800	0.68817800	-0.90203000
H	3.38495500	1.61287200	-1.66622400
C	5.69089100	-0.18298800	0.06288100
H	5.29752900	-1.48130500	1.75178800

XYZ Coordinates of the lowest energy conformer of 4e

C	7.59458400	0.01418600	-0.44930700
C	7.06129800	1.25243200	-0.03510100
N	5.73150500	1.41602000	0.17405600
C	4.92846500	0.32415400	-0.03555400
C	5.47281800	-0.92682500	-0.45554600
N	6.79721800	-1.06702100	-0.65675400
H	8.66611800	-0.12645500	-0.62010000
H	7.69274200	2.13190700	0.13519600
H	4.83048900	-1.80862700	-0.62748400
N	3.55019200	0.56081900	0.20317300
H	3.31316800	1.51894400	0.48808900
C	2.52797200	-0.40798000	0.05392000
O	2.76535000	-1.53908300	-0.32645700
C	1.17642900	0.05857100	0.37483100
C	0.70136600	1.12751400	1.09164600
S	-0.12584800	-0.92037900	-0.20898000
C	-0.73003200	1.15973100	1.16112200
H	1.31238200	1.87912100	1.57674000
C	-1.32486800	0.11165500	0.50275700
H	-1.26595700	1.93367800	1.69578200
C	-2.73716600	-0.19579400	0.33803700
C	-3.22776500	-1.47865000	0.64289900
C	-3.61080400	0.80536400	-0.12812600
C	-4.58328900	-1.77886600	0.48467500
H	-2.54998500	-2.24972300	1.01599800
C	-4.96330300	0.50957100	-0.28720500
H	-3.23264400	1.80079700	-0.36958400
C	-5.43424700	-0.77544300	0.01905800
H	-4.96363700	-2.77371400	0.72112700
F	-6.72991600	-1.02257900	-0.14446500
Cl	-6.05904800	1.69232700	-0.85130600

XYZ Coordinates of the lowest energy conformer of 4f

C	-7.24929900	0.29340200	0.03011500
C	-6.77378100	-0.98958100	0.36967300
N	-5.44673600	-1.26878700	0.39878900
C	-4.58742200	-0.24735900	0.08287400
C	-5.07469200	1.05145800	-0.25776300
N	-6.39643300	1.30596500	-0.28098800
H	-8.31757900	0.52669200	0.00352500
H	-7.44967500	-1.81373500	0.62403600
H	-4.38658200	1.87842600	-0.50773100
N	-3.21669400	-0.60516000	0.12063900
H	-3.02433700	-1.57445600	0.40095000
C	-2.14092500	0.28354700	-0.13798600
O	-2.33165300	1.45989300	-0.38417400
C	-0.80967200	-0.31957000	-0.08371000
C	-0.36842800	-1.61995900	-0.07483400
S	0.52581400	0.77747000	-0.05848700
C	1.05742300	-1.72288500	-0.03455300
H	-1.00340000	-2.49680100	-0.10342700
C	1.69758100	-0.50340700	-0.01299800
H	1.56212900	-2.68025500	-0.01921500
C	3.12386400	-0.20846700	0.01920800
C	4.05146100	-1.25894300	-0.09396600
C	3.58386100	1.11197200	0.15237100
C	5.42768000	-0.99316600	-0.07271200
H	3.70293400	-2.28326700	-0.20185600
C	4.96083900	1.37963400	0.17276000
H	2.88761300	1.94322200	0.24630600
C	5.88019400	0.32709300	0.06051000
C	5.45363800	2.78338900	0.31379300
H	6.07560600	2.90010800	1.21324200
H	6.06927800	3.07907000	-0.54829300
H	4.63975600	3.51643200	0.39090100
C	6.41506500	-2.10860500	-0.19262500
H	7.05709500	-1.97919700	-1.07628200
H	7.07594600	-2.15284700	0.68534600
H	5.93873300	-3.09310200	-0.28475500
H	6.94740800	0.53560700	0.07640800

XYZ Coordinates of the lowest energy conformer of 4g

C	7.38318200	-0.43146000	-0.22236700
C	6.93254400	0.90342500	-0.27027600
N	5.61291600	1.20910600	-0.19876400
C	4.73574400	0.16159600	-0.07705200
C	5.19772700	-1.18952300	-0.03481300
N	6.51248000	-1.46970500	-0.10602400
H	8.44534400	-0.68641300	-0.27780700
H	7.62276600	1.74894000	-0.36743600
H	4.49487100	-2.03676600	0.05223800
N	3.37508800	0.54613000	0.01553900
H	3.19855600	1.55551500	-0.06119700
C	2.28121500	-0.35769100	0.08392600
O	2.44362500	-1.56062100	0.01098800
C	0.97451000	0.27655200	0.25436100
C	0.59310700	1.49315900	0.76132900
S	-0.40983600	-0.65872400	-0.20294000
C	-0.82804600	1.67467900	0.77285000
H	1.26817300	2.25258200	1.13715400
C	-1.51692600	0.59346900	0.28089500
H	-1.29229000	2.57551400	1.15157400
C	-2.94377900	0.39224700	0.11537400
C	-3.56273900	-0.77948000	0.57905000
C	-3.72107100	1.38753100	-0.51946400
C	-4.93608800	-0.97421000	0.41709300
H	-2.97263800	-1.54871700	1.08162300
C	-5.08525600	1.21356900	-0.69257900
H	-3.23796600	2.29655800	-0.88154700
C	-5.68443900	0.02444000	-0.21925600
H	-5.70237000	1.96447200	-1.18195500
H	-5.39797800	-1.88518200	0.78319200
O	-7.03630000	-0.01444300	-0.45577700
C	-7.77196600	-1.18648500	-0.02539700
H	-7.71695500	-1.29260100	1.06171800
H	-8.79289800	-0.93635400	-0.34423200
H	-7.40753300	-2.07708400	-0.54528600

XYZ Coordinates of the lowest energy conformer of 4h

C	8.06698400	-0.51469800	-0.30128900
C	7.63955800	0.82911300	-0.27783600
N	6.32679500	1.15275600	-0.17351200
C	5.43356800	0.11535000	-0.09107300
C	5.87066600	-1.24331100	-0.12117700
N	7.17998800	-1.54194000	-0.22398500
H	9.12410300	-0.78450900	-0.38360700
H	8.34366100	1.66646500	-0.34309700
H	5.15502900	-2.08240300	-0.06621300
N	4.08021800	0.52013100	0.03980500
H	3.92232400	1.53538100	0.01430100
C	2.97403900	-0.36565800	0.07304900
O	3.10758600	-1.56645400	-0.06435000
C	1.67695400	0.28004200	0.29460800
C	1.32318800	1.47097600	0.87720100
S	0.27615900	-0.60416900	-0.20178400
C	-0.09532500	1.67574600	0.90644200
H	2.01420200	2.19438600	1.29316100
C	-0.80073800	0.63517500	0.35402200
H	-0.54407600	2.56219200	1.33666800
C	-2.23982300	0.47703900	0.19108400
C	-2.88501900	-0.68225100	0.65500200
C	-2.98400300	1.49303900	-0.43610800
C	-4.26323300	-0.82553100	0.49030800
H	-2.31586400	-1.46812300	1.15302600
C	-4.36062500	1.34808600	-0.60085700
H	-2.48225500	2.38996500	-0.79928200
C	-5.00176800	0.18770500	-0.13758900
H	-4.94788100	2.13179900	-1.08951400
H	-4.77380800	-1.72461900	0.84890800
C	-6.46775400	0.07211000	-0.33163600
O	-7.22239800	0.86731700	-0.84318900
O	-6.92164600	-1.12983200	0.17335700
C	-8.34531200	-1.39135000	0.04779200
H	-8.46303500	-2.32690100	0.60457700
H	-8.91752800	-0.57225200	0.49563400
H	-8.59890500	-1.50902900	-1.01038900

XYZ Coordinates of the lowest energy conformer of 4i

C	-7.75344000	-0.55599100	0.02078000
C	-7.31930000	0.59109500	0.71612800
N	-6.00448900	0.91350200	0.80001500
C	-5.11573500	0.07467800	0.17730400
C	-5.56050900	-1.08927500	-0.52071700
N	-6.87102900	-1.38953900	-0.59214400
H	-8.81180900	-0.82233700	-0.05306900
H	-8.01920300	1.26908400	1.21745700
H	-4.84819600	-1.77368600	-1.01435700
N	-3.76087600	0.47869400	0.28075400
H	-3.59806300	1.32484900	0.84035800
C	-2.65706600	-0.26166600	-0.21755600
O	-2.80243100	-1.35110900	-0.73864400
C	-1.35637700	0.39108300	-0.06531100
C	-0.98788700	1.69104500	0.17471800
S	0.03786500	-0.61684800	-0.26236600
C	0.43329200	1.86923400	0.21862400
H	-1.67104800	2.52034100	0.31220900
C	1.13010300	0.70487000	0.00986900
H	0.89147600	2.83131100	0.40756300
C	2.56606600	0.47564500	-0.02187800
C	3.15716700	-0.47838400	0.82123500
C	3.37223000	1.22101900	-0.90458600
C	4.53877100	-0.69106000	0.78338700
H	2.54361800	-1.05262500	1.51608000
C	4.74829800	1.00800600	-0.94628000
H	2.91403500	1.96088400	-1.56124800
C	5.32464500	0.04996400	-0.09907400
H	5.36484000	1.58570900	-1.63711700
H	4.97753800	-1.43332400	1.44776200
S	7.06609800	-0.10840800	-0.24512100
C	7.54894900	-1.46191000	0.84257300
H	7.07341300	-2.41047500	0.56763800
H	8.63660900	-1.58883200	0.73297400
H	7.34235200	-1.24663800	1.89703500

XYZ Coordinates of the lowest energy conformer of 4j

C	-7.21953900	0.28941700	0.14729800
C	-6.73913300	-0.55489800	-0.87533700
N	-5.41180200	-0.77050700	-1.04992600
C	-4.55780800	-0.13204700	-0.18751200
C	-5.04836400	0.72616500	0.84210700
N	-6.37142800	0.92516600	0.99826700
H	-8.28881900	0.46760000	0.29616400
H	-7.41176700	-1.07040800	-1.57037400
H	-4.36491400	1.25142300	1.53226000
N	-3.18554400	-0.41852100	-0.40802200
H	-2.99005100	-1.03274600	-1.20842800
C	-2.11523900	0.17707500	0.30378800
O	-2.29992800	1.03697200	1.14377800
C	-0.78396200	-0.33140200	-0.04179600
C	-0.35921700	-1.49037800	-0.64179800
S	0.55925300	0.65452000	0.41909500
C	1.06829300	-1.57237900	-0.74143500
H	-1.00400200	-2.28309900	-1.00177300
C	1.70649500	-0.47534900	-0.21653900
H	1.57124600	-2.41772100	-1.19446200
C	3.13512900	-0.19543500	-0.13276000
C	3.98521000	-1.12789200	0.48679600
C	3.65250700	0.99671800	-0.66594300
C	5.34965600	-0.83564600	0.55911400
H	3.58201600	-2.05006400	0.90586700
C	5.02738900	1.22714100	-0.56063500
H	3.00027600	1.71904700	-1.15835200
C	5.91523500	0.33510700	0.04641500
H	6.98378000	0.53999700	0.11633100
F	5.51832900	2.35608400	-1.06713400
F	6.15446200	-1.71855900	1.14649100

XYZ Coordinates of the lowest energy conformer of 4k

C	-7.35705400	0.01995400	-0.32814700
C	-6.78106200	-1.26728900	-0.32492100
N	-5.44109600	-1.44318900	-0.21230300
C	-4.67116400	-0.31368800	-0.10092900
C	-5.25863300	0.98753400	-0.11045300
N	-6.59220000	1.13887200	-0.22203300
H	-8.43701700	0.17066400	-0.41702600
H	-7.38560500	-2.17713000	-0.41332500
H	-4.64252700	1.90050100	-0.03180400
N	-3.28216600	-0.56581700	0.03645800
H	-3.01044500	-1.55605300	-0.00587800
C	-2.28314900	0.43830300	0.10080400
O	-2.55143400	1.61901300	-0.01256400
C	-0.92339100	-0.06072900	0.32151600
C	-0.44070200	-1.22327200	0.86879700
S	0.36983300	0.99692700	-0.12190100
C	0.98981400	-1.26463200	0.92043200
H	-1.04935300	-2.03646300	1.24632000
C	1.58156100	-0.13046900	0.41465600
H	1.52747500	-2.10903900	1.33393600
C	2.96400600	0.20567500	0.28508300
C	3.61838000	1.38248500	0.53255100
S	4.08894400	-1.01236900	-0.27947100
C	5.03362700	1.31938900	0.27237800
H	3.14961700	2.28851700	0.89940300
C	5.43559800	0.09369300	-0.16938600
H	5.68672900	2.17056500	0.42208300
Cl	6.99961300	-0.37572800	-0.57767000

XYZ Coordinates of the lowest energy conformer of 4l

C	-7.01179600	0.06400200	-0.20954600
C	-6.44640300	-1.22402000	-0.30405800
N	-5.10500100	-1.41541200	-0.24241700
C	-4.32257000	-0.30013900	-0.08324600
C	-4.90041000	1.00304300	0.00631400
N	-6.23491100	1.16953500	-0.05604800
H	-8.09236900	0.22693100	-0.25677700
H	-7.06040300	-2.12268700	-0.43137200
H	-4.27422300	1.90499600	0.12396800
N	-2.93304700	-0.56795100	-0.00353300
H	-2.66994300	-1.55500600	-0.11455200
C	-1.92299000	0.42466800	0.09652900
O	-2.18913100	1.61114600	0.06742700
C	-0.56322300	-0.09447800	0.24360400
C	-0.07047500	-1.30439700	0.66590100
S	0.72508100	0.99998800	-0.12290200
C	1.35956900	-1.35158800	0.68478800
H	-0.67299300	-2.15048400	0.97435000
C	1.94700000	-0.17453000	0.27983500
H	1.90207500	-2.23322700	1.00238900
C	3.32505600	0.17112400	0.15458600
C	3.95824000	1.37692700	0.28560100
S	4.49434700	-1.07659100	-0.23680500
C	5.38206700	1.30819700	0.07361700
H	3.47011400	2.31204200	0.53409600
C	5.83510000	0.05528700	-0.21794800
H	6.00539700	2.18919200	0.14781600
C	7.19313000	-0.42876500	-0.49673600
H	7.52278200	-1.18407600	0.23624300
H	7.27238300	-0.89116700	-1.49493200
H	7.93632300	0.38478900	-0.46680300

XYZ Coordinates of the lowest energy conformer of 4m

C	8.64659600	0.13220100	-0.37496600
C	8.18822100	0.14515200	0.95921800
N	6.86625000	0.08148600	1.25356300
C	5.99559200	0.00293300	0.19706600
C	6.46316400	-0.00364500	-1.15098800
N	7.78176800	0.05921100	-1.42070200
H	9.71173100	0.18155600	-0.62140400
H	8.87476200	0.20760700	1.81141900
H	5.76630300	-0.05519200	-2.00592700
N	4.62964900	-0.08644100	0.57429100
H	4.45146800	-0.03827000	1.58530400
C	3.54523900	-0.09818300	-0.33527400
O	3.70581100	0.02004900	-1.53489900
C	2.22427900	-0.27780300	0.27859900
C	1.82228000	-0.79276000	1.48431000
S	0.86282300	0.18208900	-0.68486900
C	0.39579100	-0.79841400	1.63789900
H	2.48131100	-1.17362200	2.25567100
C	-0.26161700	-0.28984400	0.54646600
H	-0.08961000	-1.16641000	2.53332600
C	-1.69266200	-0.13223800	0.32584400
C	-2.26522800	1.15068200	0.27743500
C	-2.49977600	-1.26881200	0.16435900
C	-3.64066300	1.28567100	0.06428800
H	-1.62356100	2.02694400	0.41347300
C	-3.87778000	-1.12063300	-0.04788600
H	-2.04388000	-2.26357700	0.20291500
C	-4.45371500	0.15308100	-0.10035200
H	-5.52920400	0.27673600	-0.26735900
C	-4.28930500	2.64459400	0.00761200
C	-4.71268400	-2.36341200	-0.21557700
F	-4.92075200	2.89734300	-1.15085700
F	-3.47371700	3.69868500	0.16257100
F	-5.23486800	2.83287500	0.94351000
F	-6.02703600	-2.17702800	-0.40769200
F	-4.65908300	-3.19614000	0.83805000
F	-4.34243700	-3.12915700	-1.25543900

XYZ Coordinates of the lowest energy conformer of 4n

C	-8.28880300	-0.08264400	0.32772600
C	-7.80689200	-0.60070700	-0.89260400
N	-6.47855500	-0.67410700	-1.15472200
C	-5.62513600	-0.22369400	-0.18037700
C	-6.11736100	0.30554800	1.05018000
N	-7.44152800	0.36814000	1.29011300
H	-9.35891500	-0.02139100	0.54810700
H	-8.47925700	-0.96376500	-1.67840200
H	-5.43526900	0.68042000	1.83342600
N	-4.24960000	-0.35256400	-0.50638700
H	-4.05601900	-0.72583100	-1.44403300
C	-3.18567300	0.11700900	0.30150500
O	-3.38143300	0.72370000	1.33746100
C	-1.84219500	-0.19798200	-0.19522600
C	-1.37566600	-1.10680000	-1.11106500
S	-0.53829100	0.68814800	0.51627000
C	0.05073300	-1.07295200	-1.25033900
H	-1.98847300	-1.79755200	-1.67805300
C	0.64742800	-0.13951400	-0.43852900
H	0.58033600	-1.71935500	-1.93916400
C	2.05850900	0.18612200	-0.29214200
C	2.49578000	1.51768800	-0.39122300
C	2.98778800	-0.84079500	-0.04913200
C	3.85638000	1.79125600	-0.24164700
H	1.78840400	2.32678700	-0.59068500
C	4.34761900	-0.53596300	0.09463800
H	2.63766500	-1.87339600	0.03276700
C	4.79762800	0.78582800	0.00135800
H	5.85367500	1.04563400	0.11265100
C	5.31045100	-1.66774300	0.35268300
F	6.60577400	-1.33638100	0.46413100
F	5.30587600	-2.61190000	-0.60434200
F	5.05766100	-2.34952400	1.48266700
Cl	4.39543600	3.41944000	-0.36215300