

Synthesis of coumarin and homoisoflavonoid derivatives and analogs: The search for new antifungal agents

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Table S1. Results of docking **compound 8** to its potential targets.

Target	Pose	PLP ^(a)	Z_PLP ^(b)	GS ^(c)	Z_GS ^(d)	CS ^(e)	Z_CS ^(f)	ASP ^(g)	Z_ASP ^(h)	Aggregated Score
GRE3	1	52.29	1.27	5.93	0.87	20.72	1.83	33.37	2.02	1.50
	2	52.96	1.41	-0.08	0.22	19.28	1.31	32.2	1.68	1.16
	1	50.41	2.2	12.79	0.73	14.3	-0.21	30.99	2.01	1.18
ALD2	2	49.17	1.92	7.58	0.41	17.28	0.92	28.7	1.25	1.12
	3	43.27	0.59	21.4	1.26	17.83	1.12	28.2	1.08	1.01
	1	46.31	0.33	19.95	2.18	17.83	0.67	36.03	2.43	1.4
GCY1	2	47.28	0.63	13.8	1.71	18.43	0.99	29.07	0.87	1.05
	3	46.81	0.48	-6.42	0.16	20.3	1.99	31.99	1.53	1.04
	1	42.24	2.4	-28.15	0.43	10.25	1.75	17.71	1.31	1.47
ARA1	2	37.82	1.34	1.24	1.45	8.02	1.14	18.84	1.56	1.37
	3	34.84	0.63	-0.06	1.4	6.87	0.82	18.37	1.46	1.08
	1	67.85	1.33	26.67	0.67	26.92	0.98	39.54	1.14	1.03
ALD1	1	74.91	3.73	-3.66	-1.31	27.29	2.41	35.39	2.12	1.74
	2	61.93	0.87	11.17	0.03	27.65	2.57	34.33	1.73	1.3
	1	46.41	0.96	10.6	0.66	16.17	1.26	24.04	1.16	1.01
UGA2	1	53.41	2.07	26.35	1.19	13.25	2.07	15.34	0.74	1.52
	2	51.15	1.48	22.29	0.78	10.33	0.53	19.06	2.16	1.24
	3	53.06	1.98	23.89	0.94	11.92	1.37	12.76	-0.25	1.01
ERG1	1	50.34	1.19	7.73	0.87	25.34	1.54	27.51	1.13	1.18
	2	50.27	1.18	4.65	0.79	23.44	1.12	27.02	1.05	1.04
	1	59.4	1.43	33.17	1.13	25.32	1.77	32.55	0.32	1.16
BTS1	2	59.38	1.42	30.27	0.94	24.93	1.47	32.74	0.42	1.06
	3	61.3	2.32	9.73	-0.39	24.83	1.4	33.42	0.75	1.02
	1	68.52	2.48	35.96	1.74	26.69	1.16	34.39	1.65	1.76
HST2	2	62.57	1.05	21.8	0.37	27.67	1.65	32.45	1.09	1.04

(a) PLP score, (b) Scaled PLP score, (c) GoldScore score, (d) Scaled GoldScore score, (e) ChemScore score, (f) Scaled ChemScore score, (g) ASP score, (h) Scaled ASP score

Table S2. Predicted free energies of binding of **compound 8** to its potential targets and its components according to the MM-PBSA method. Energy values are expressed as kcal/mol.

Target	Conformer	MM-PBSA Component							ΔG
		VD WAALS	EEL	EPB	ENPOLAR	EDISPER	ΔG gas	ΔG solv.	TOTAL
GRE3	1	-22.02	-3.17	16.40	-16.95	29.58	-25.19	29.03	3.85
	2	-26.41	-3.80	15.66	-19.79	33.34	-30.21	29.21	-1.00
ALD2	1	-15.18	-4.22	11.02	-12.63	21.21	-19.40	19.60	0.20
	2	-15.94	-3.88	11.39	-12.62	21.40	-19.83	20.16	0.34
	3	-21.57	-9.05	15.62	-17.15	26.70	-30.62	25.18	-5.44
GCY1	1	-30.87	-18.53	31.05	-23.66	38.31	-49.41	45.71	-3.70
	2	-32.59	-6.64	23.39	-24.45	38.54	-39.23	37.48	-1.75
	3	-32.27	-7.35	23.35	-24.47	38.69	-39.62	37.56	-2.05
ARA1	1	-24.81	-4.99	16.09	-19.14	31.52	-29.81	28.47	-1.34
	2	-23.87	-1.66	13.69	-18.54	30.68	-25.53	25.82	0.29
	3	-28.84	-15.57	24.06	-22.82	36.08	-44.41	37.31	-7.10
ALD5	1	-35.50	-16.13	30.33	-24.99	41.68	-51.63	47.02	-4.61
ALD1	1	-37.92	-20.77	40.69	-27.05	44.92	-58.69	58.56	-0.13
	2	-34.99	-26.01	43.57	-25.17	42.73	-61.00	61.13	0.13
UGA2	1	-36.62	-8.22	30.32	-26.40	44.87	-44.83	48.79	3.96
	1	-34.46	-20.66	48.42	-22.40	39.38	-55.12	65.40	10.28
FBA1	2	-38.12	-12.21	41.92	-24.85	42.79	-50.33	59.86	9.54
	3	-26.55	-24.91	73.57	-18.72	32.73	-51.45	87.58	36.13
ERG1	1	-36.00	-2.55	18.50	-27.34	46.52	-38.54	37.68	-0.86
	2	-36.43	-20.97	32.57	-27.45	46.13	-57.39	51.25	-6.14
BTS1	1	-39.01	-8.61	26.66	-27.01	43.53	-47.62	43.18	-4.44
	2	-37.78	-3.52	32.61	-27.21	45.86	-41.30	51.25	9.95
	3	-37.94	-6.22	33.97	-26.96	45.55	-44.17	52.56	8.39
HST2	1	-37.90	-14.08	33.59	-26.77	44.70	-51.98	51.52	-0.46
	2	-33.08	-2.09	19.50	-24.42	40.12	-35.17	35.21	0.03

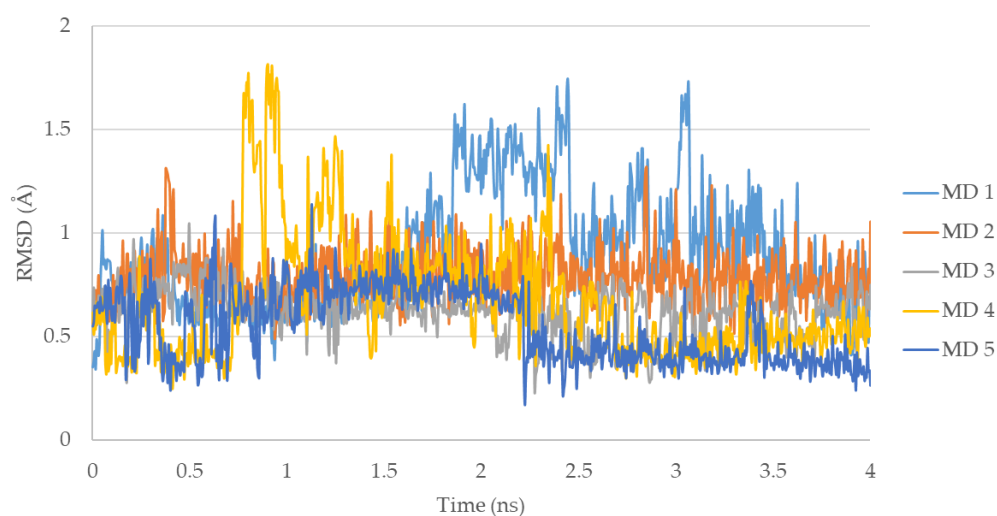


Figure S1. Ligand RMSD vs. time for the ALD1-compound 8 complex (docking pose 1).

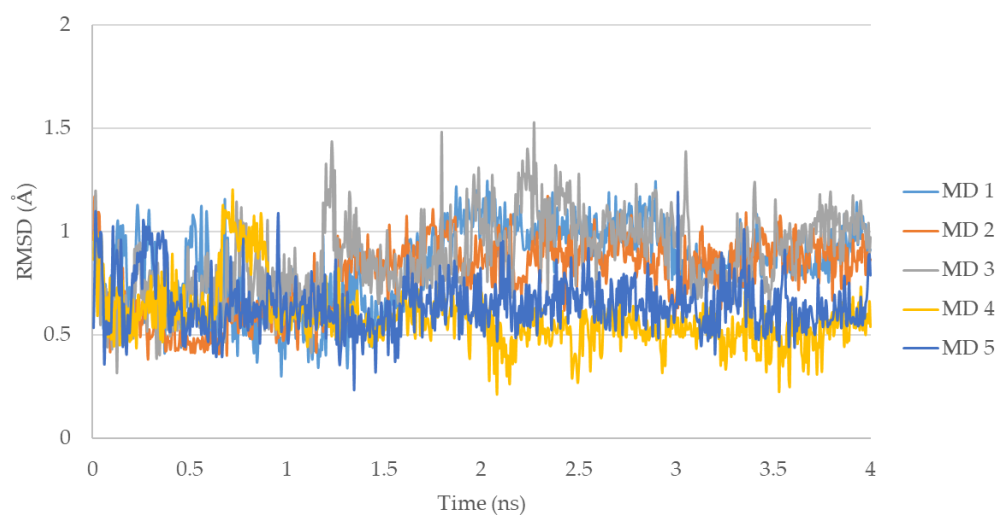


Figure S2. Ligand RMSD vs. time for the ALD1-compound 8 complex (docking pose 2).

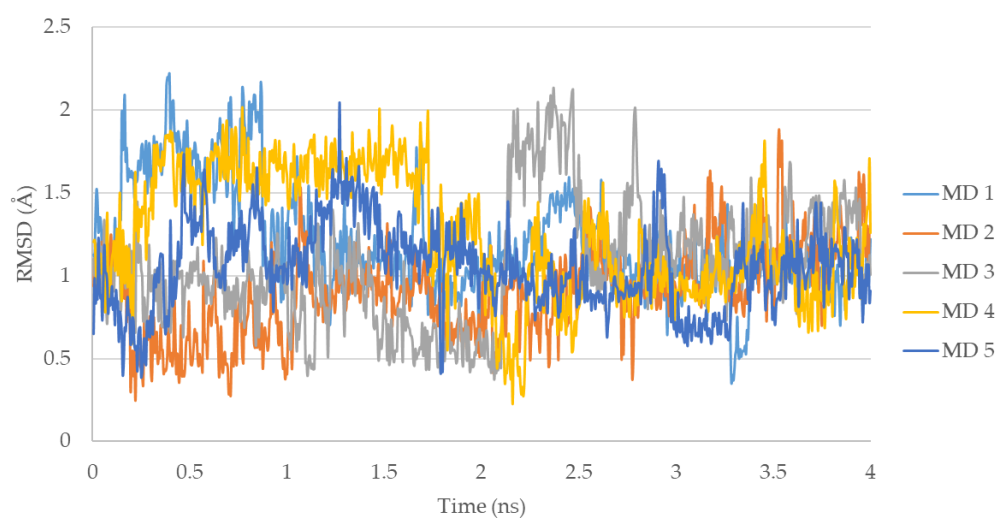


Figure S3. Ligand RMSD vs. time for the ALD2-compound 8 complex (docking pose 1).

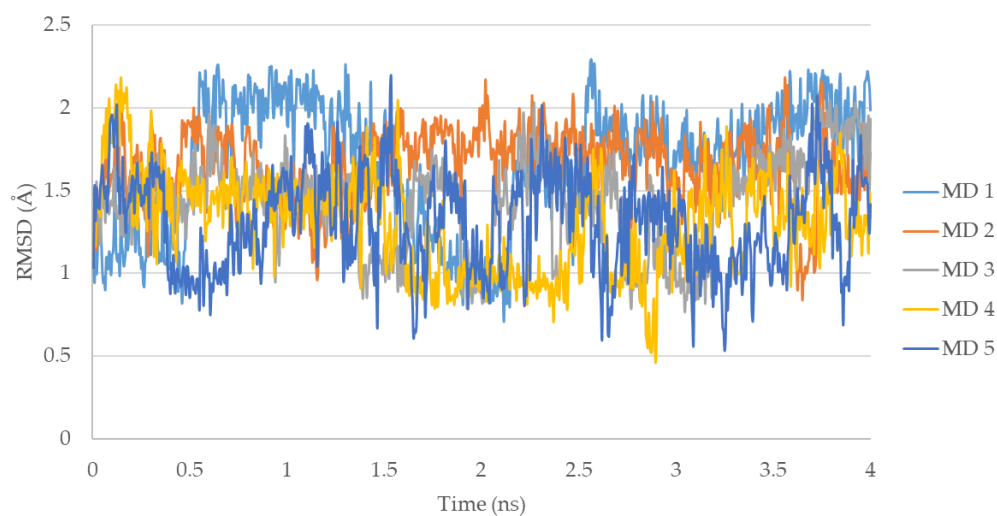


Figure S4. Ligand RMSD vs. time for the ALD2-compound 8 complex (docking pose 2).

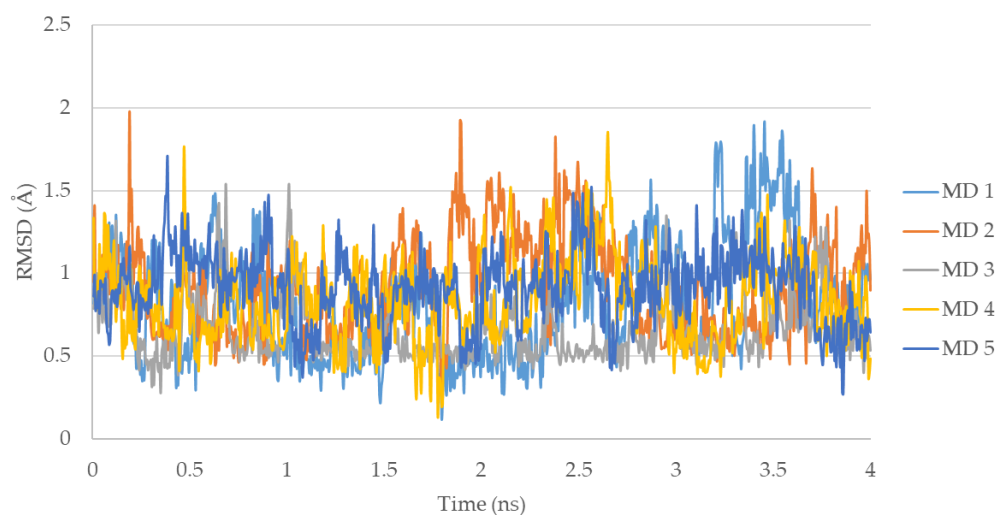


Figure S5. Ligand RMSD vs. time for the ALD2-compound **8** complex (docking pose 3).

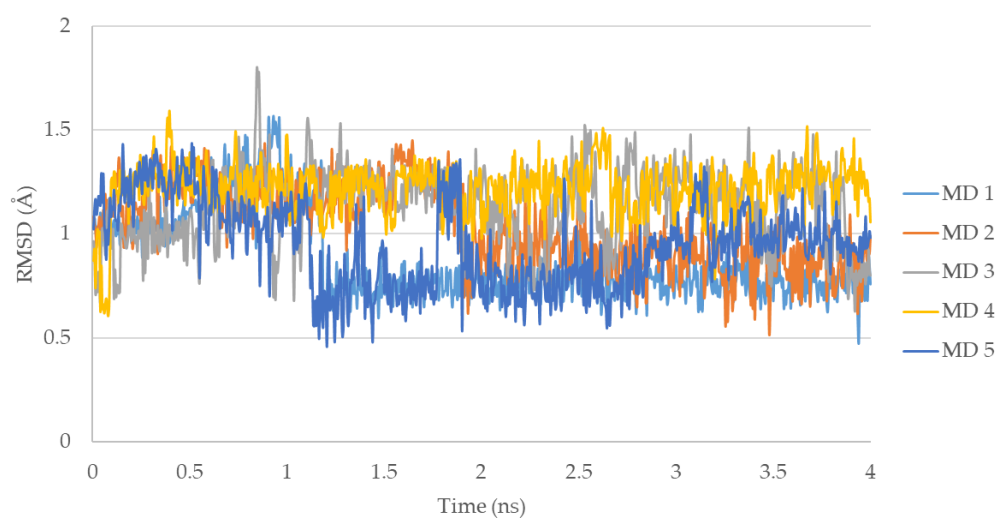


Figure S6. Ligand RMSD vs. time for the ALD5-compound **8** complex (docking pose 1).

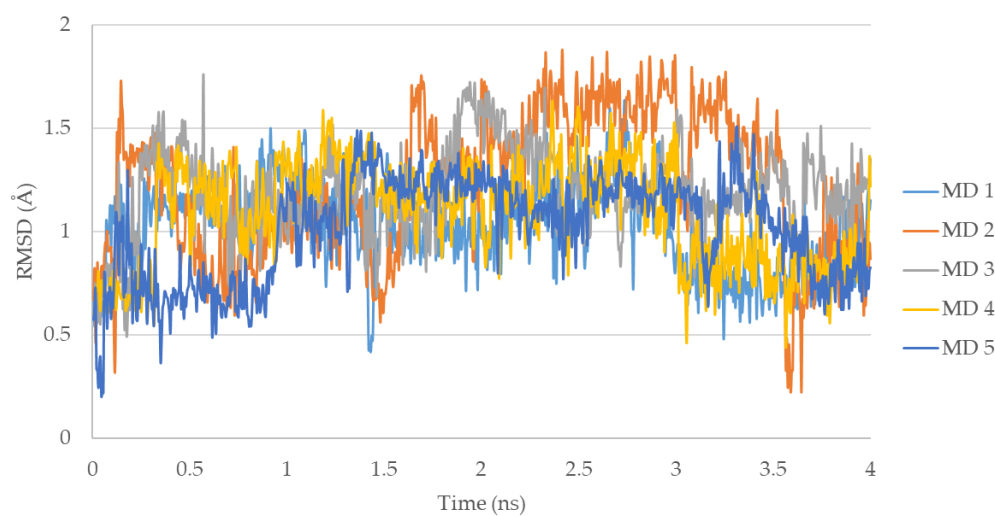


Figure S7. Ligand RMSD vs. time for the ARA1-compound **8** complex (docking pose 1).

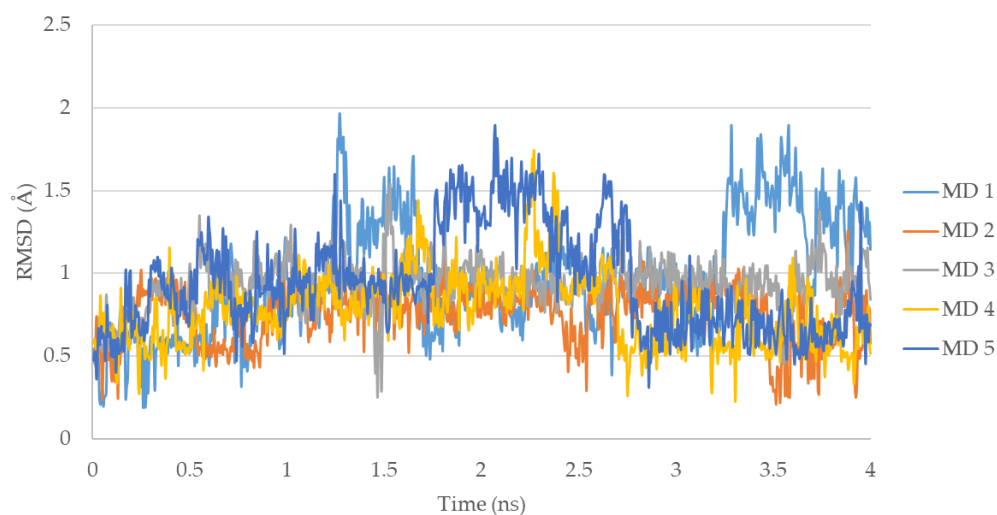


Figure S8. Ligand RMSD vs. time for the ARA1-compound 8 complex (docking pose 2).

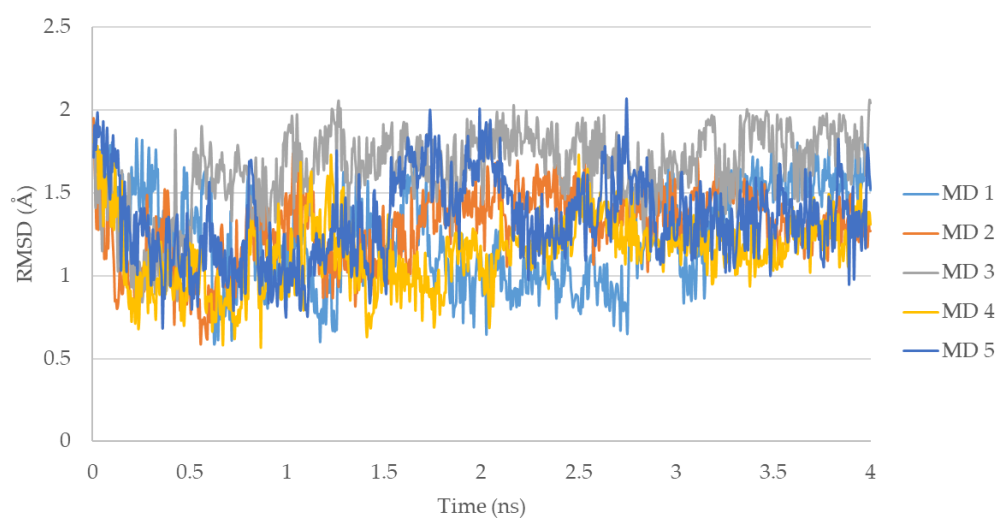


Figure S9. Ligand RMSD vs. time for the ARA1-compound 8 complex (docking pose 3).

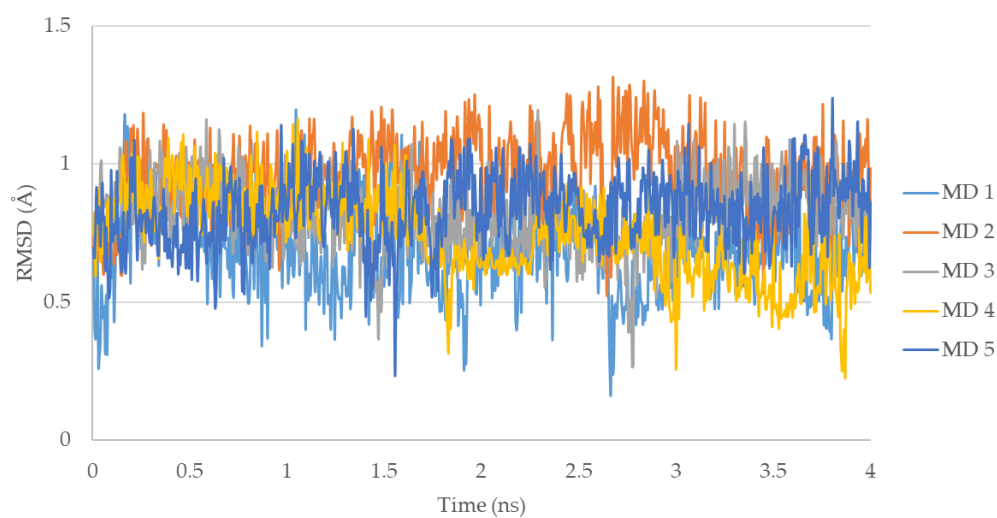


Figure S10. Ligand RMSD vs. time for the BTS1-compound 8 complex (docking pose 1).

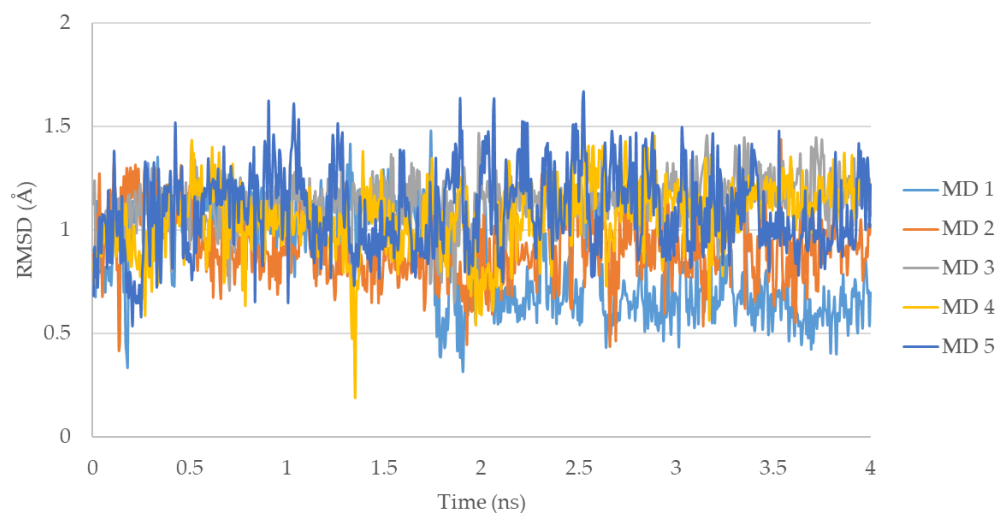


Figure S11. Ligand RMSD vs. time for the BTS1-compound 8 complex (docking pose 2).

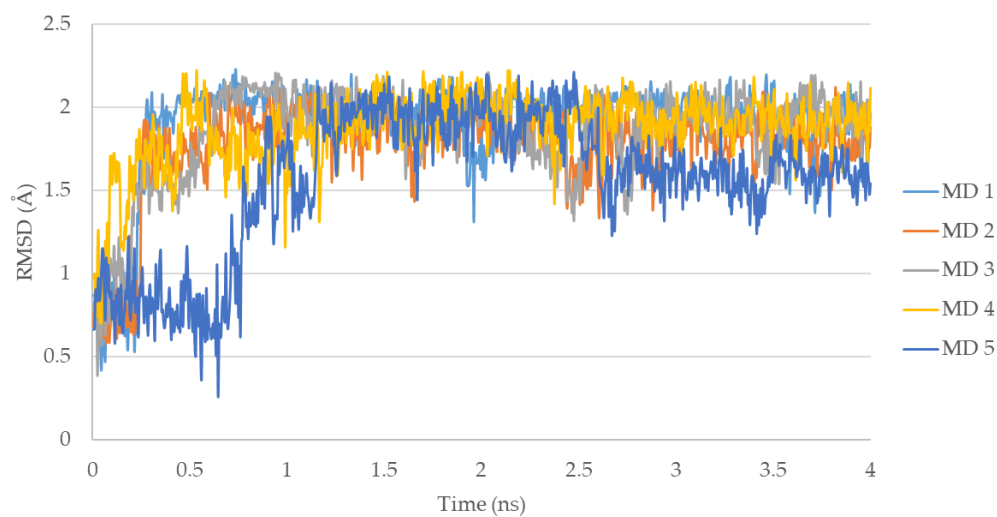


Figure S12. Ligand RMSD vs. time for the BTS1-compound 8 complex (docking pose 3).

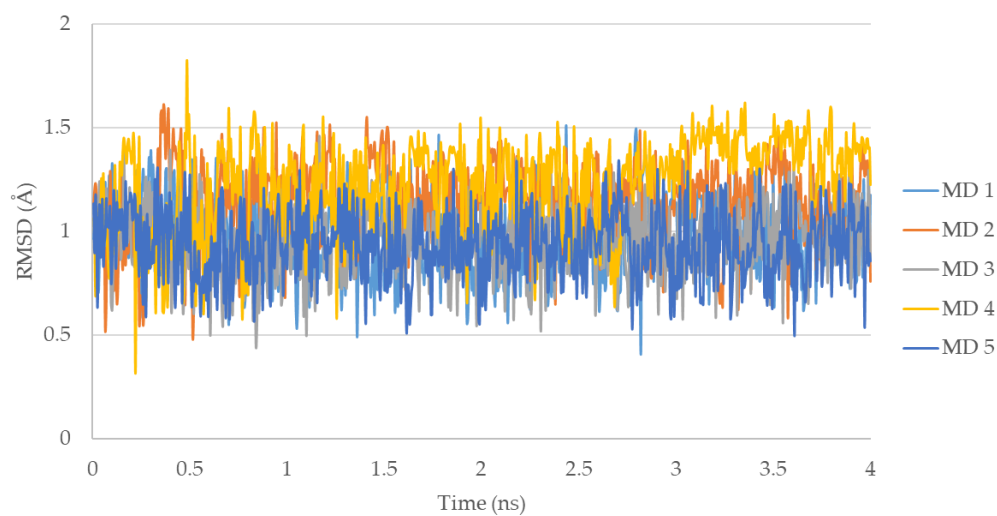


Figure S13. Ligand RMSD vs. time for the ERG1-compound 8 complex (docking pose 1).

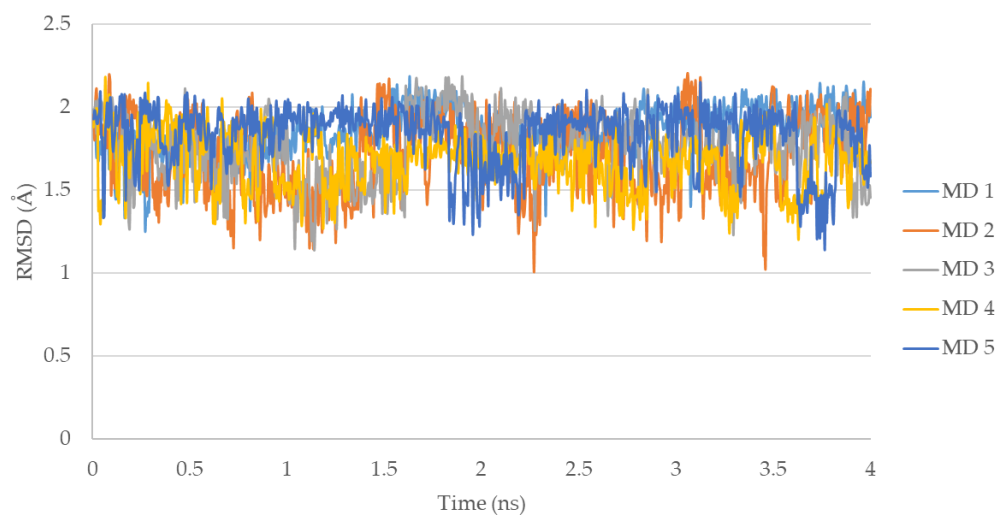


Figure S14. Ligand RMSD vs. time for the ERG1-compound 8 complex (docking pose 2).

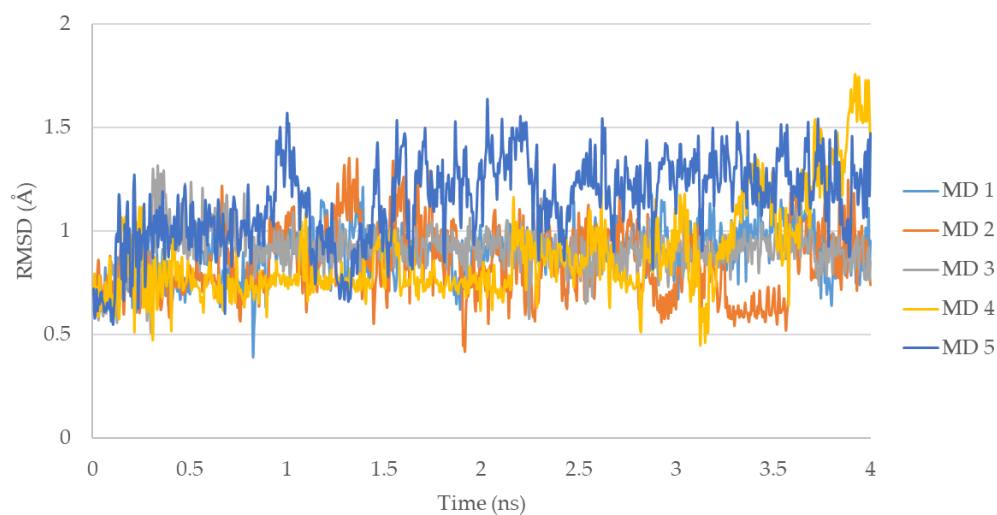


Figure S15. Ligand RMSD vs. time for the FBA1-compound 8 complex (docking pose 1).

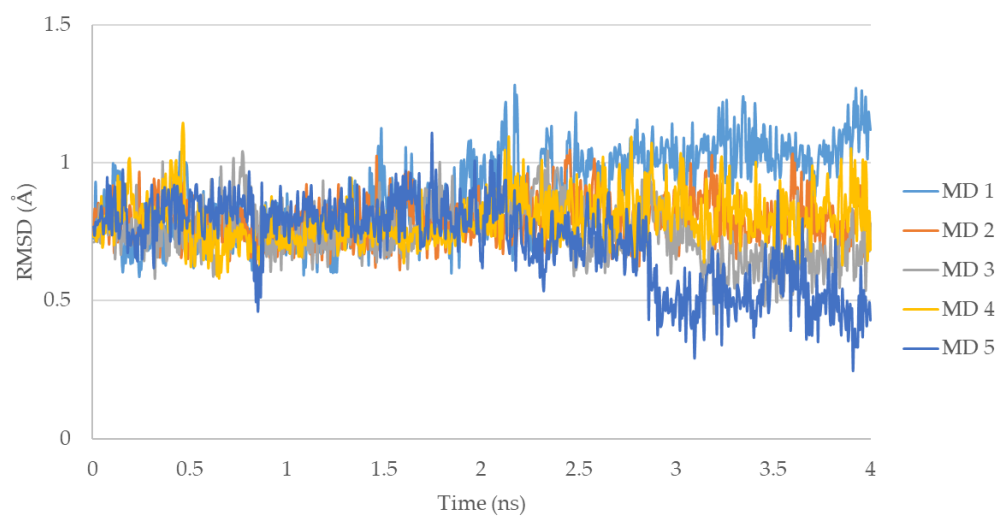


Figure S16. Ligand RMSD vs. time for the FBA1-compound 8 complex (docking pose 2).

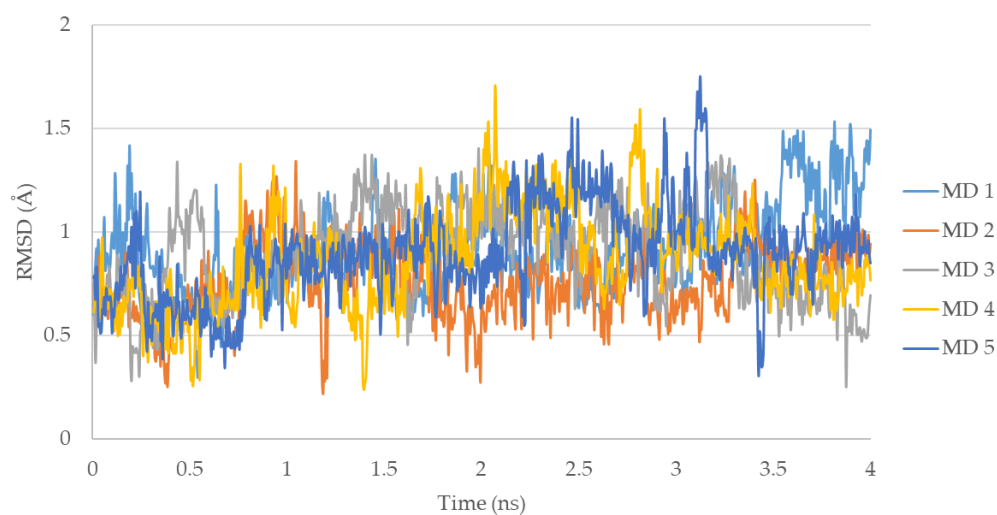


Figure S17. Ligand RMSD vs. time for the FBA1-compound 8 complex (docking pose 3).

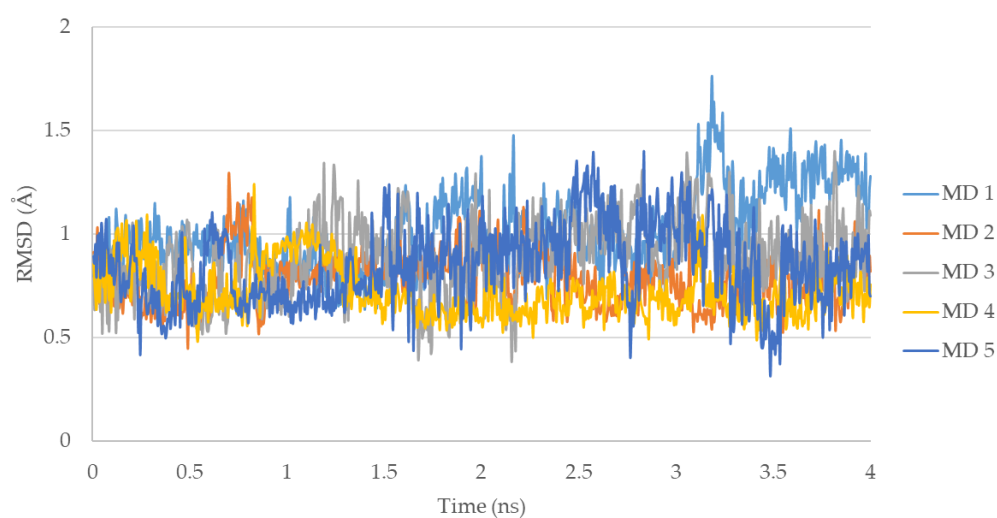


Figure S18. Ligand RMSD vs. time for the GCY1-compound 8 complex (docking pose 1).

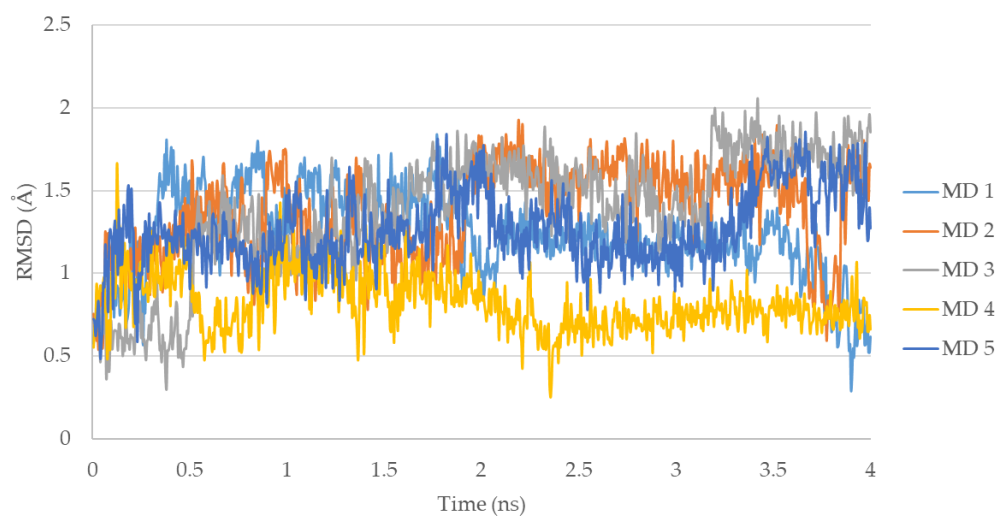


Figure S19. Ligand RMSD vs. time for the GCY1-compound 8 complex (docking pose 2).

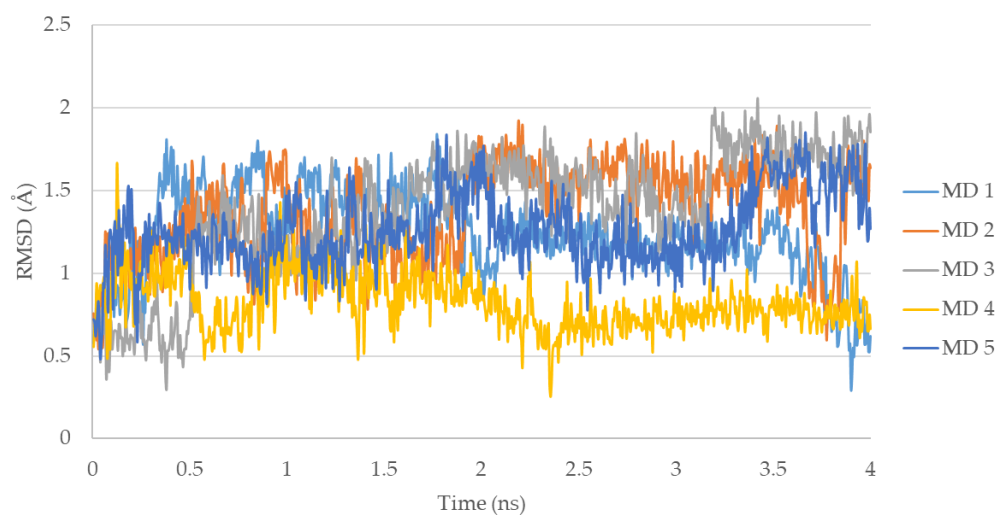


Figure S20. Ligand RMSD vs. time for the GCY1-compound 8 complex (docking pose 3).

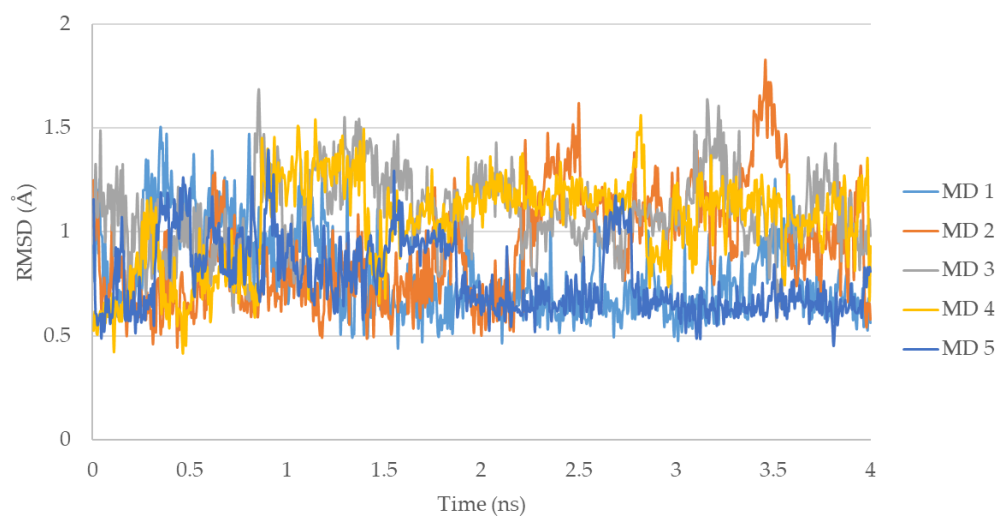


Figure S21. Ligand RMSD vs. time for the GRE3-compound 8 complex (docking pose 1).

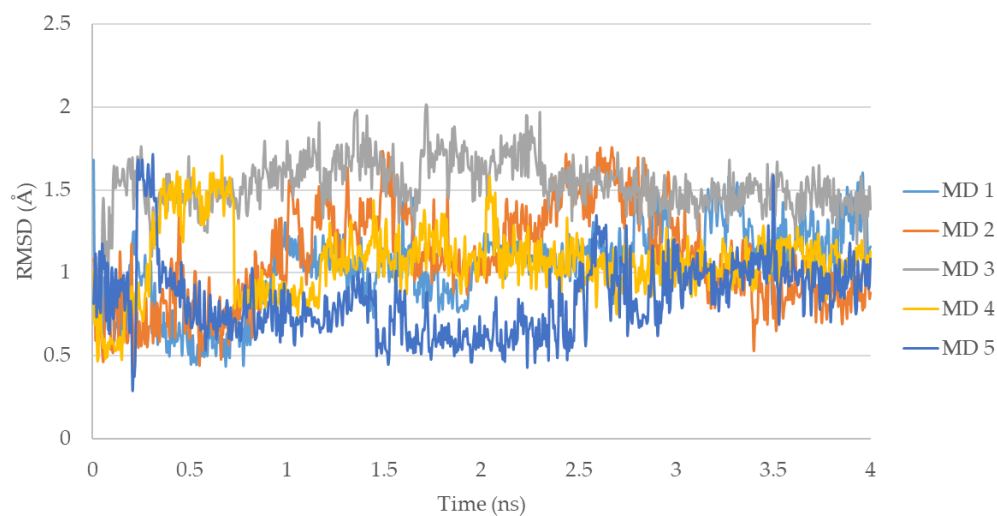


Figure S22. Ligand RMSD vs. time for the GRE3-compound 8 complex (docking pose 2).

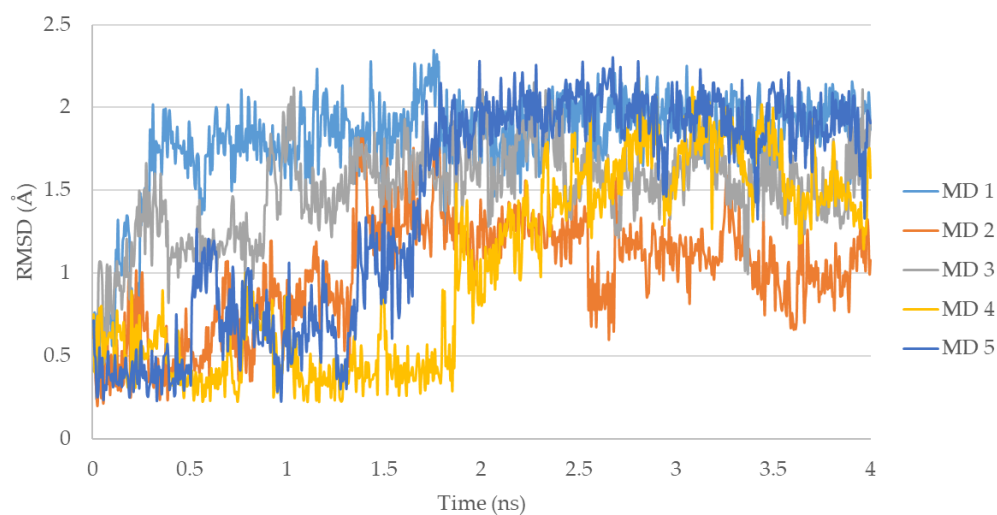


Figure S23. Ligand RMSD vs. time for the HTS2-compound 8 complex (docking pose 1).

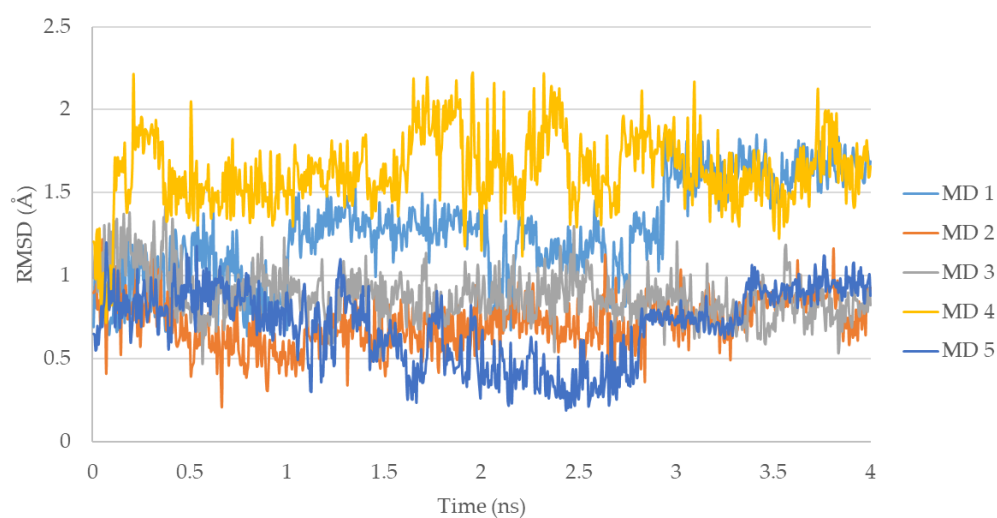


Figure S24. Ligand RMSD vs. time for the HTS2-compound 8 complex (docking pose 2).

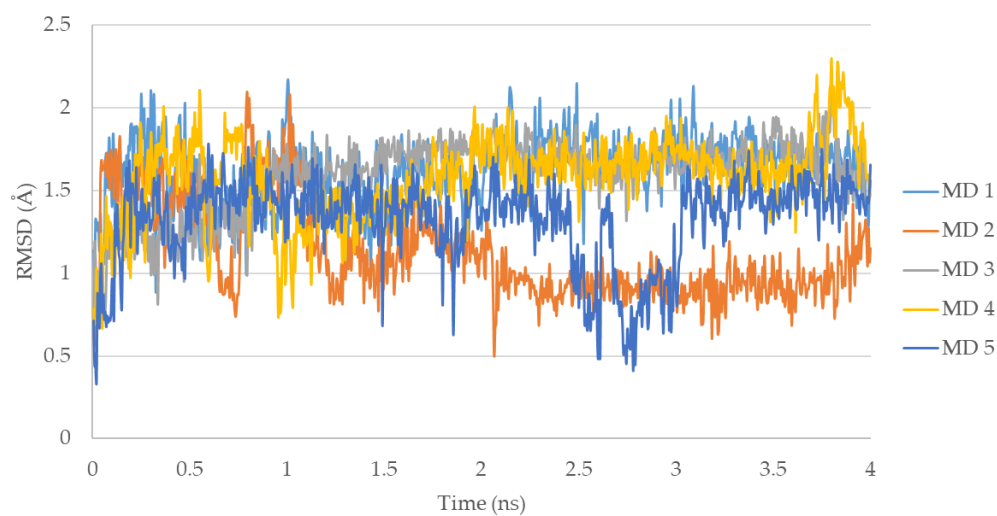
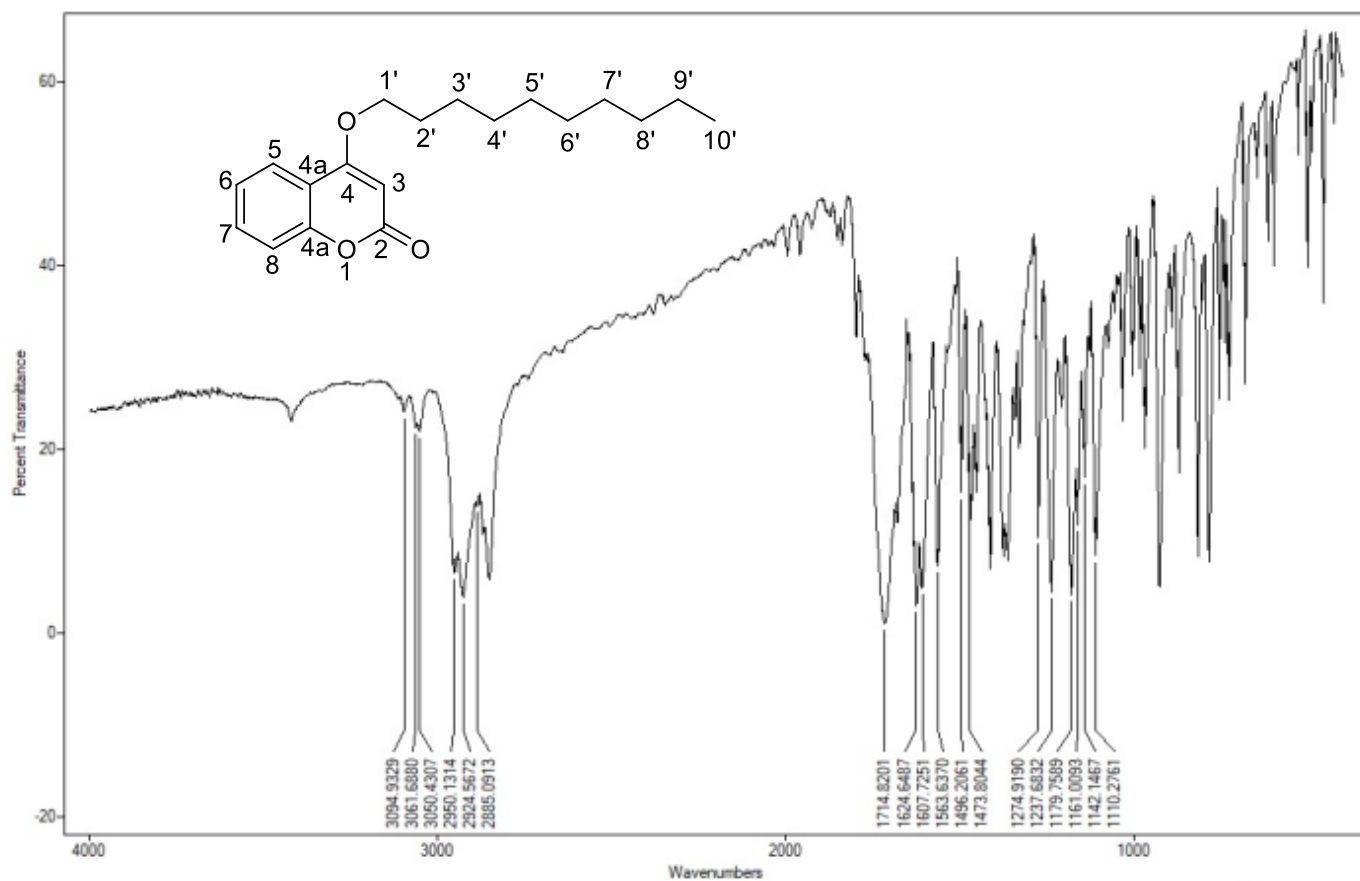
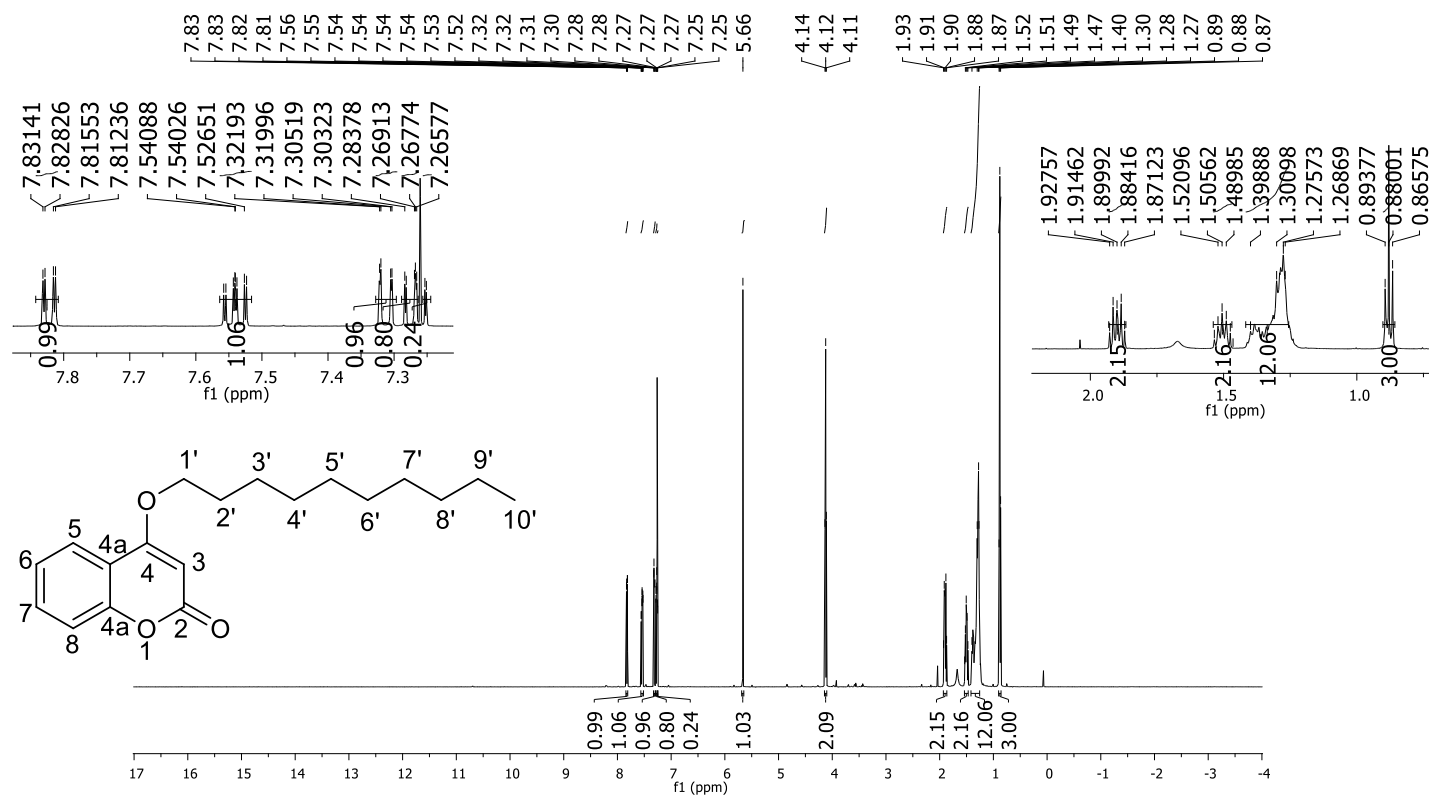


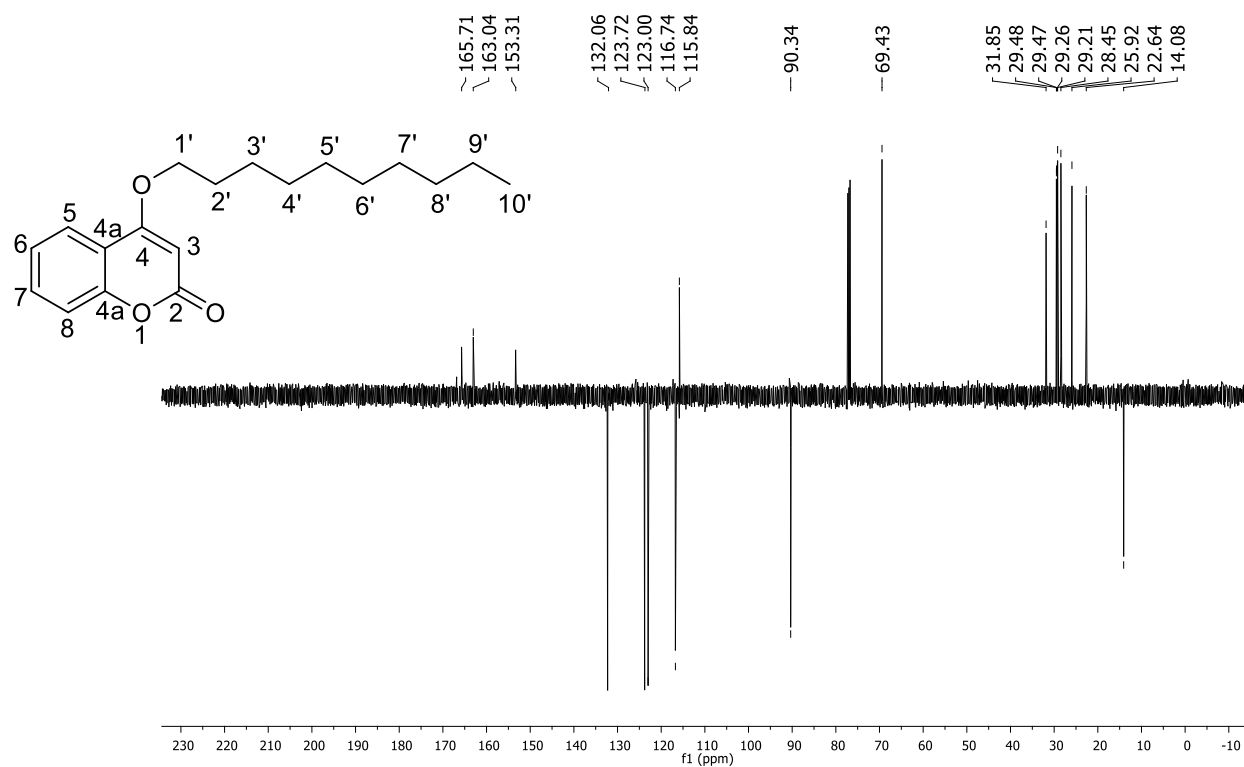
Figure S25. Ligand RMSD vs. time for the UGA2-compound 8 complex (docking pose 1).



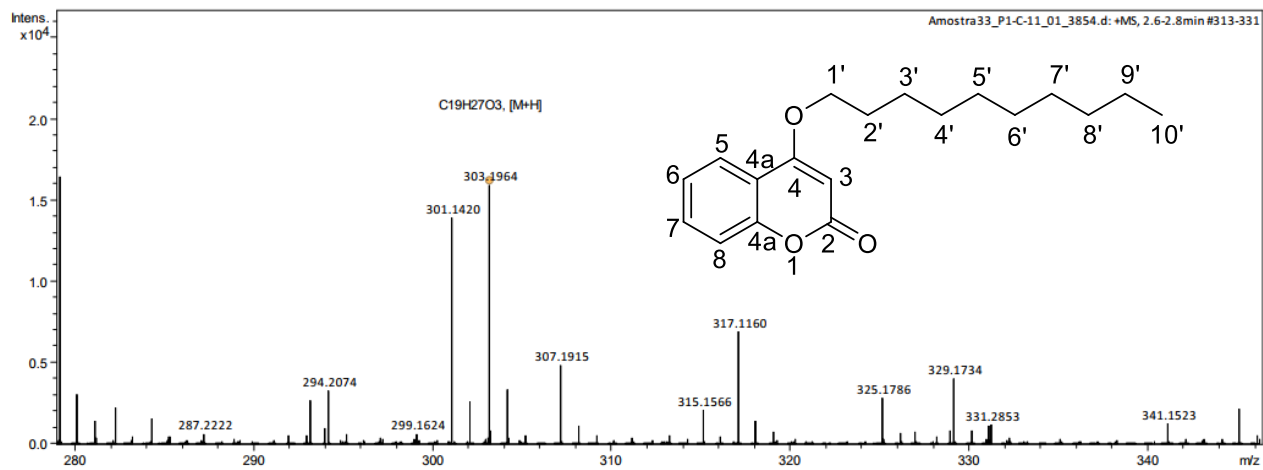
Spectrum S1. Infrared spectrum ν_{\max} (KBr, cm^{-1}) of compound **3**.



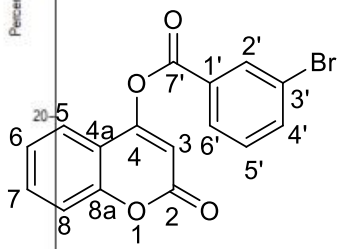
Spectrum S2. ^1H NMR spectrum (500 MHz, CDCl_3) of compound **3**.



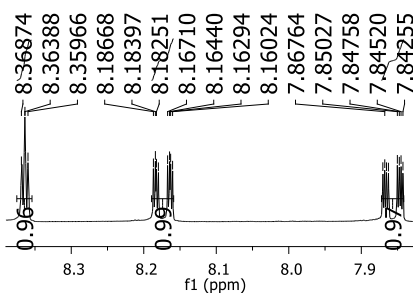
Spectrum S3. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 3.



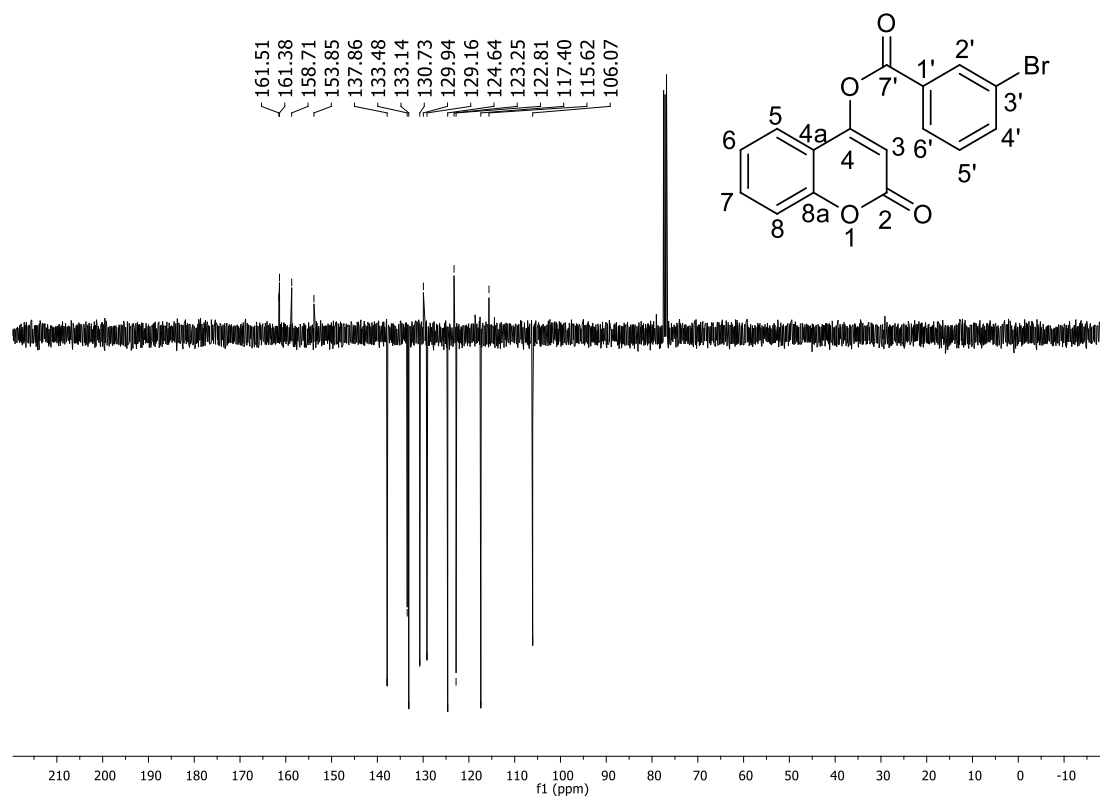
Spectrum S4. HRMS spectrum of compound 3.



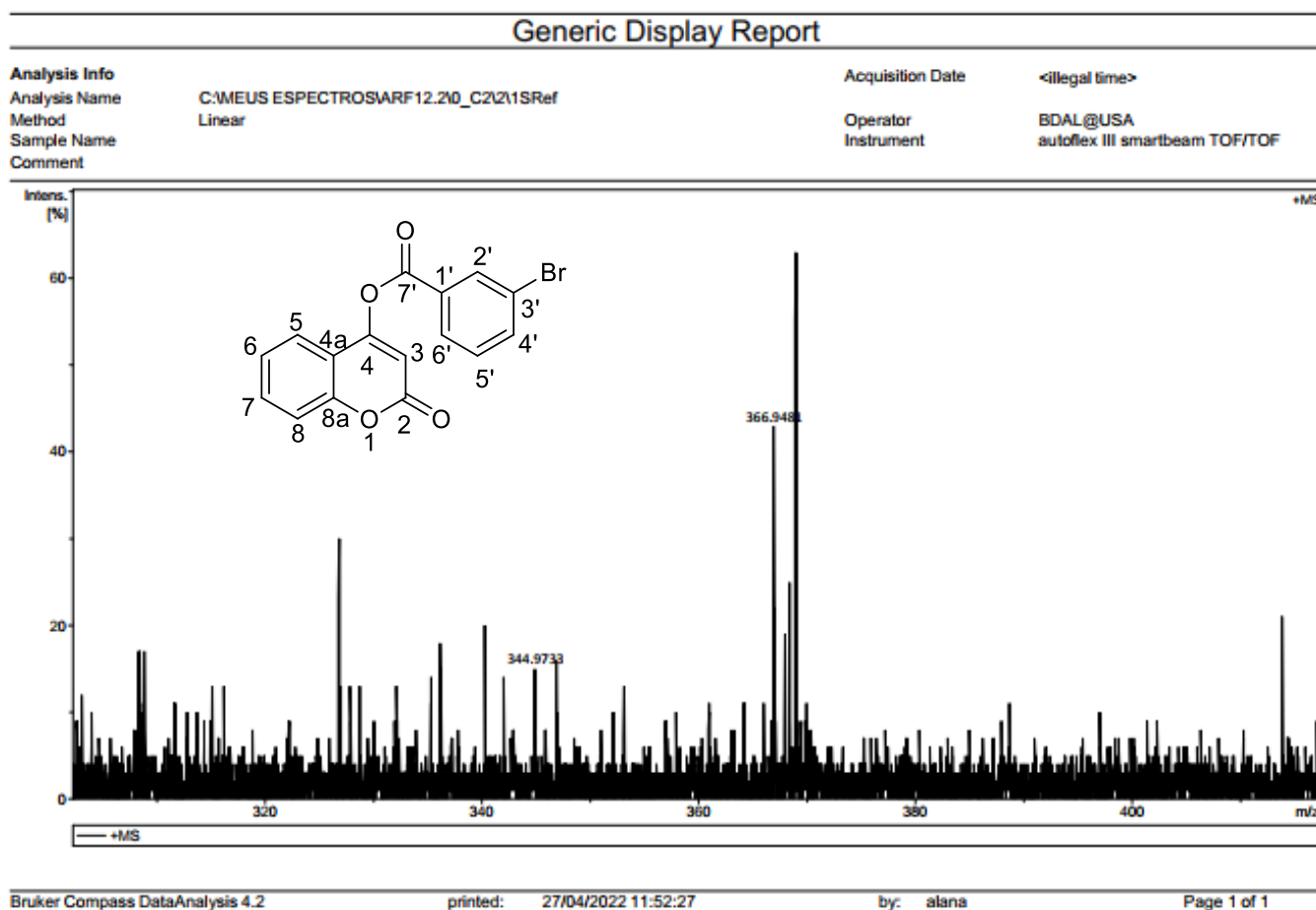
8.37	8.36	8.36	8.19	8.18	8.18	8.18	8.17	8.16	8.16	8.16	7.68	7.68	7.67	7.66	7.62	7.62	7.62	7.62	7.60	7.60	7.49	7.49	7.47	7.46	7.45	7.43	7.43	7.41	7.40	7.35	7.35	7.33	7.33	7.33	7.31	7.31	6.60
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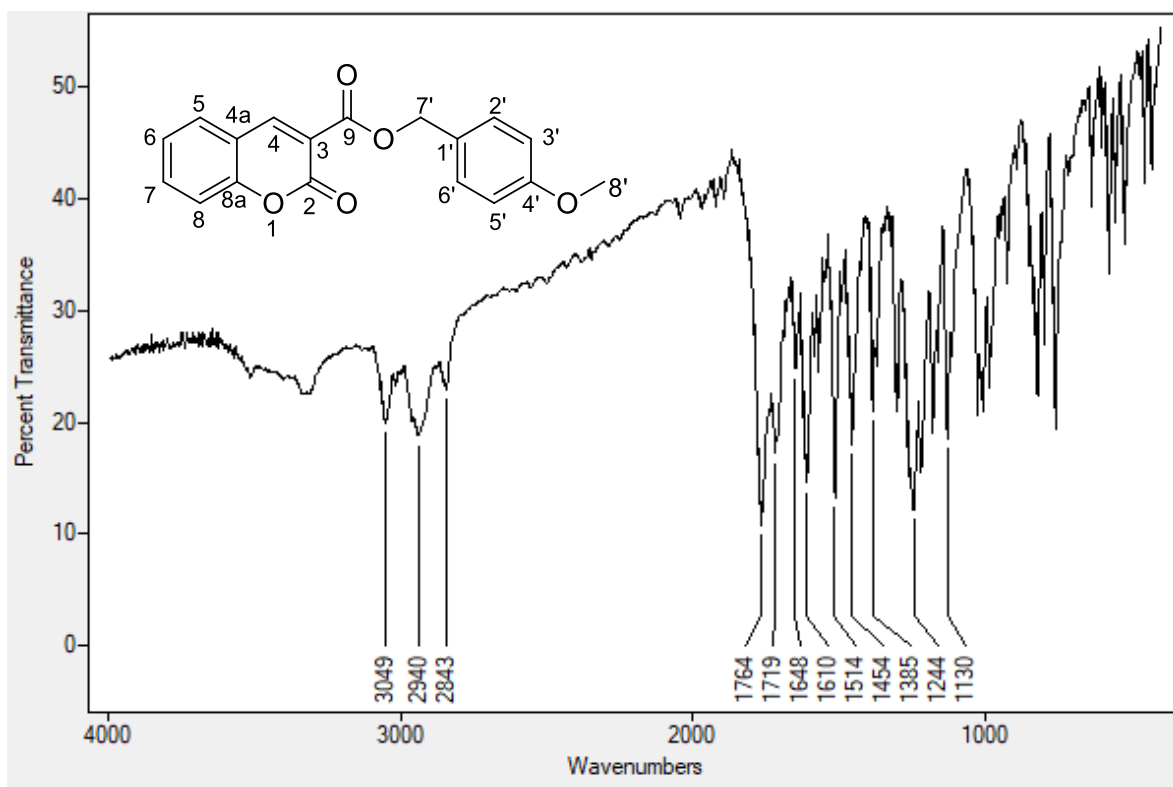
Spectrum S6. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **4**.



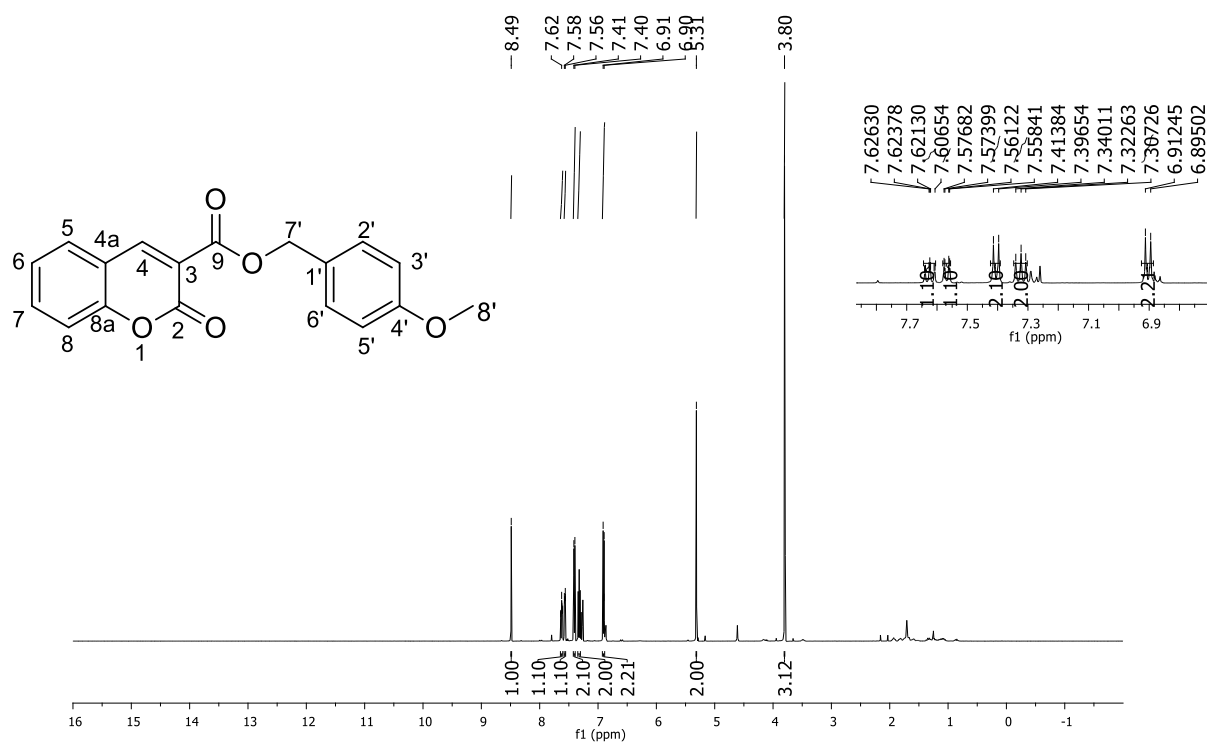
Spectrum S7. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound 4.



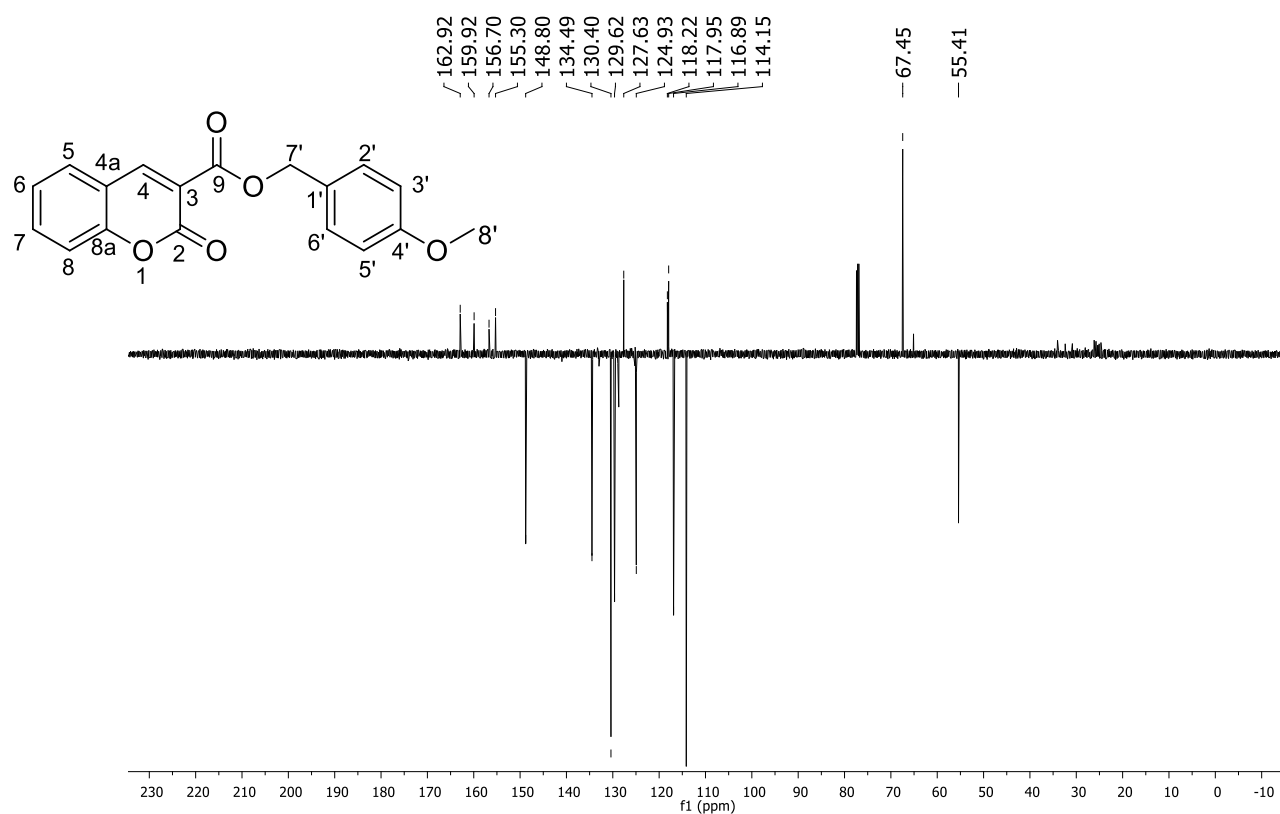
Spectrum S8. HRMS spectrum of compound 4.



Spectrum S9. Infrared spectrum ν_{\max} (KBr, cm⁻¹) of compound 10 .



Spectrum S10. ¹H NMR spectrum (500 MHz, CDCl₃) of compound 10.



Spectrum S11. ¹³C NMR spectrum (125 MHz, CDCl₃) of compound 10.

Analysis Info

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 Sample Name:
 Comment:

Acquisition Date

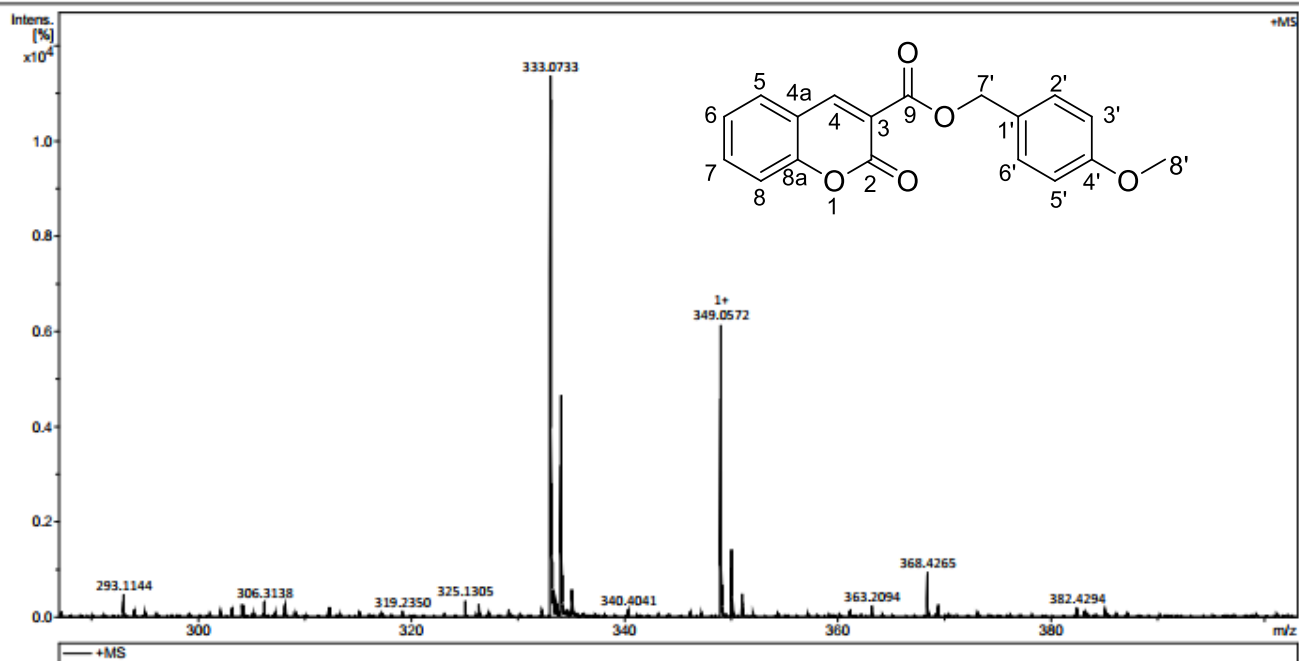
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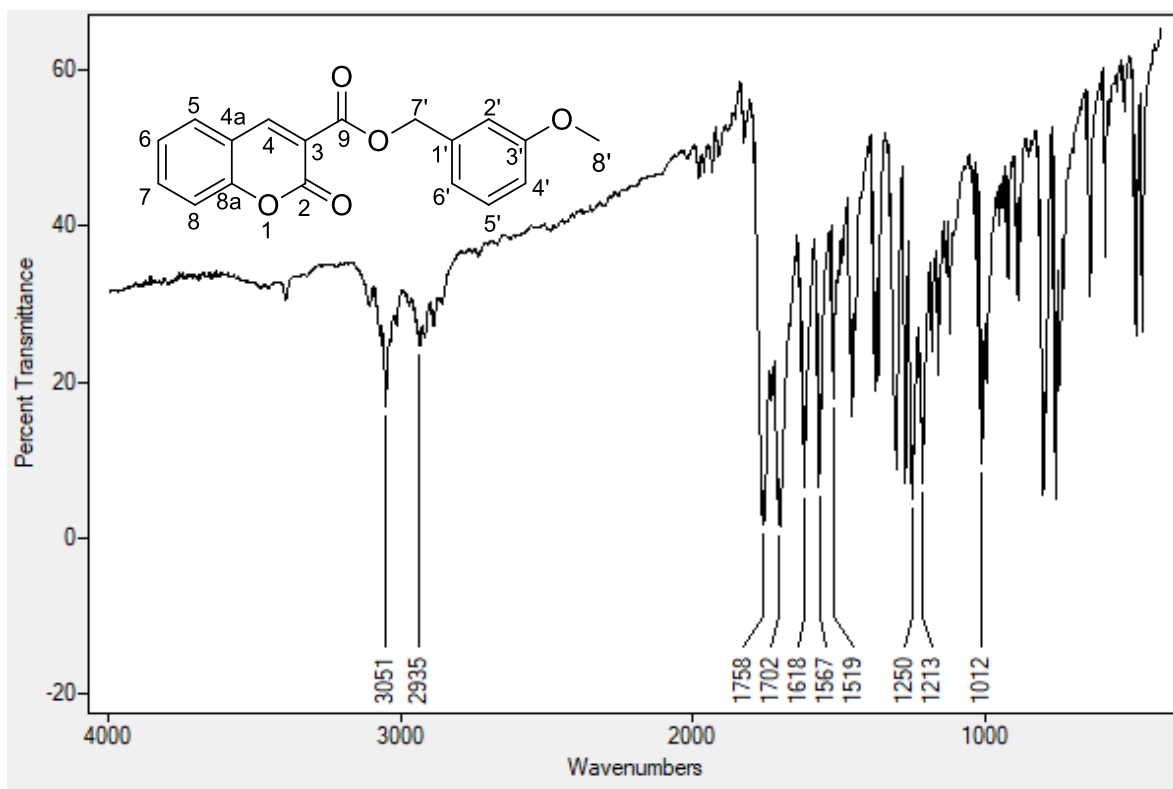
BDAL@USA

Instrument

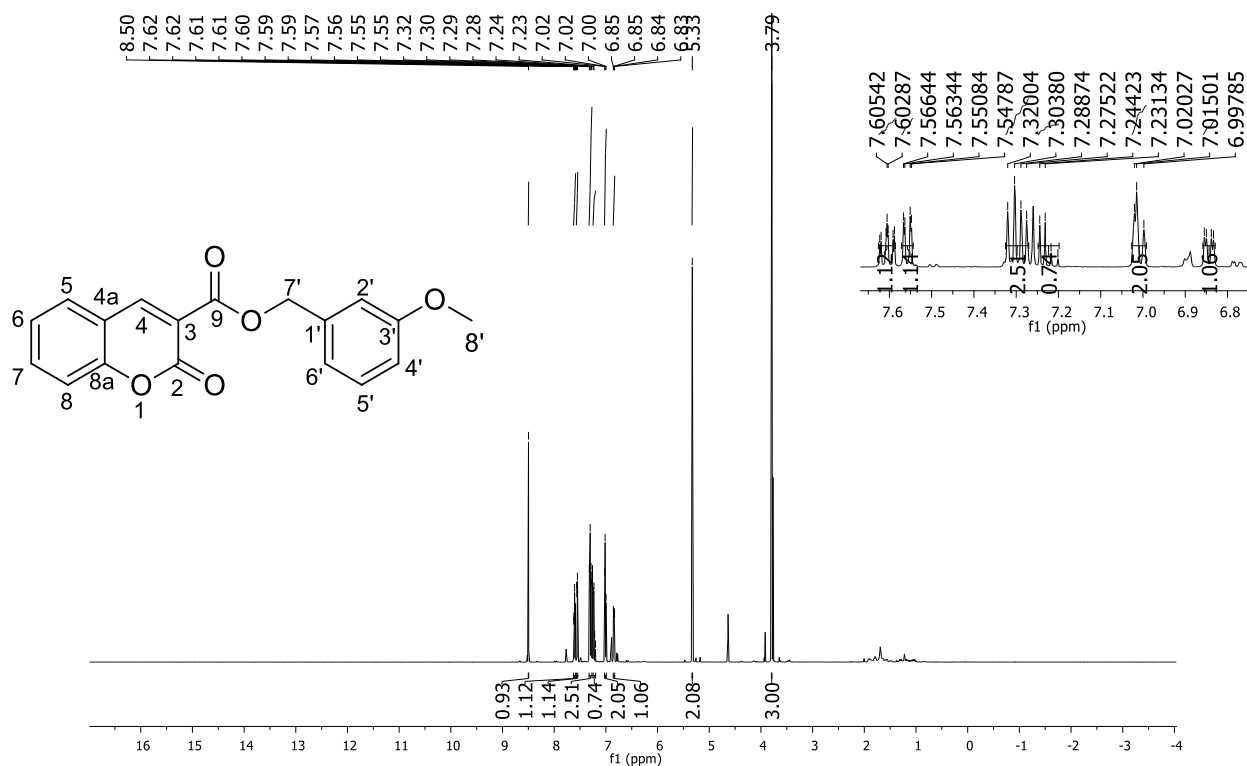
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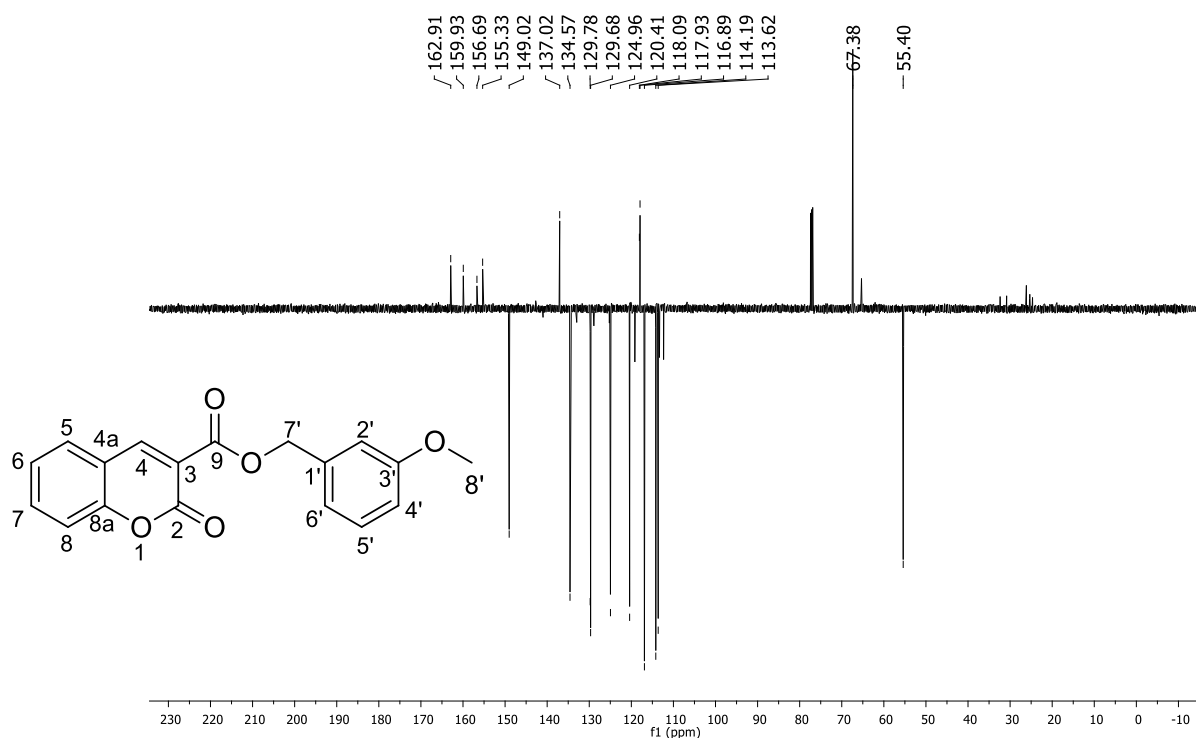


Spectrum S12. HRMS spectrum of compound 10.

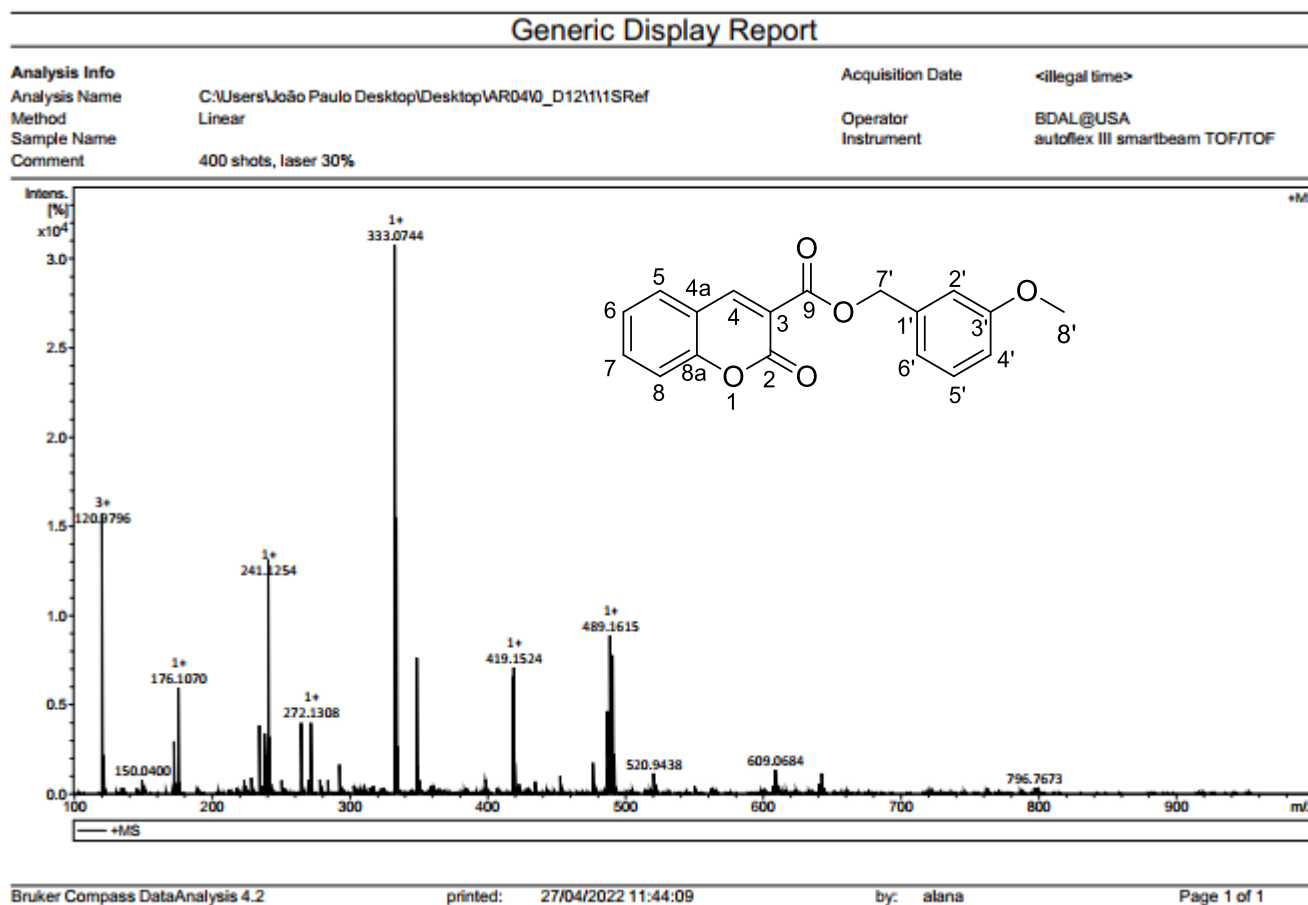


Spectrum S13. Infrared sprectra ν_{max} (KBr, cm^{-1}) of compound **11**.

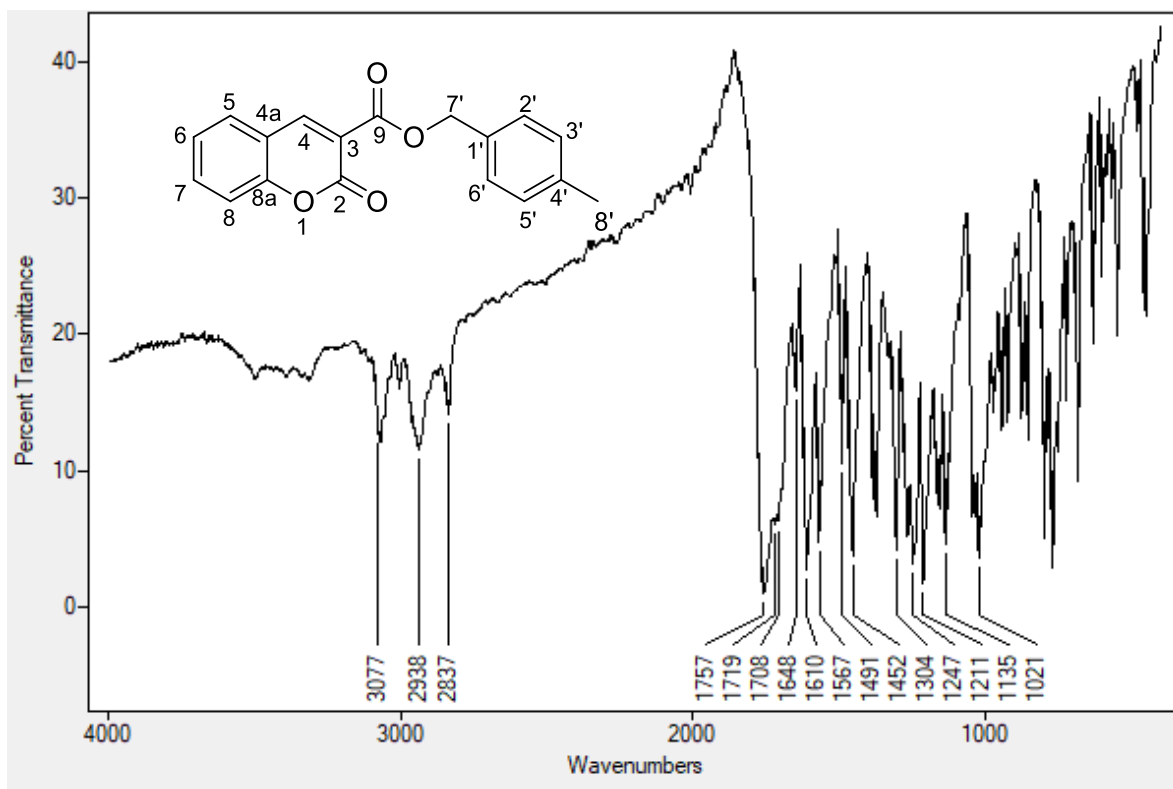




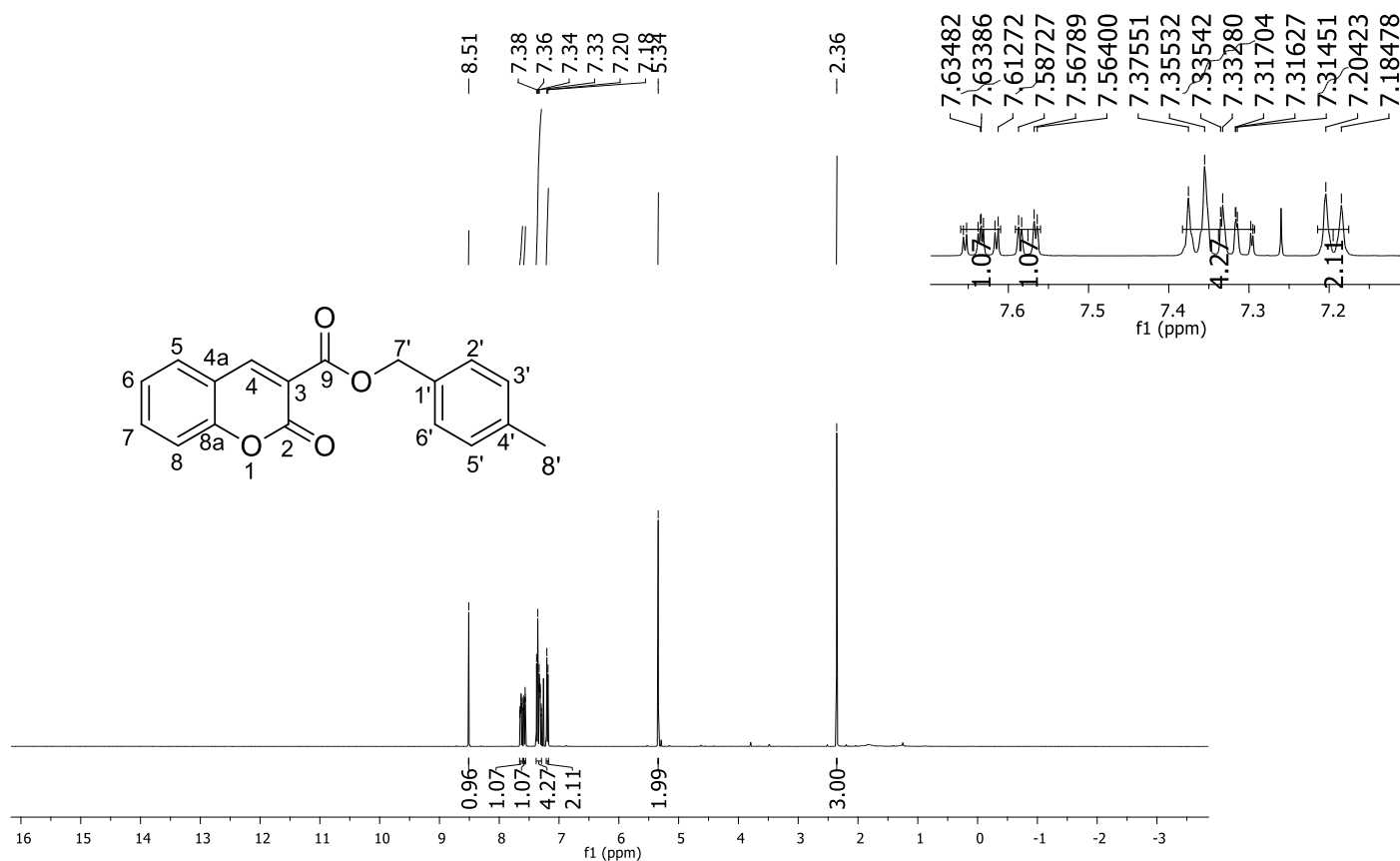
Spectrum S15. ¹³C NMR spectrum (125 MHz, CDCl₃) of 11.

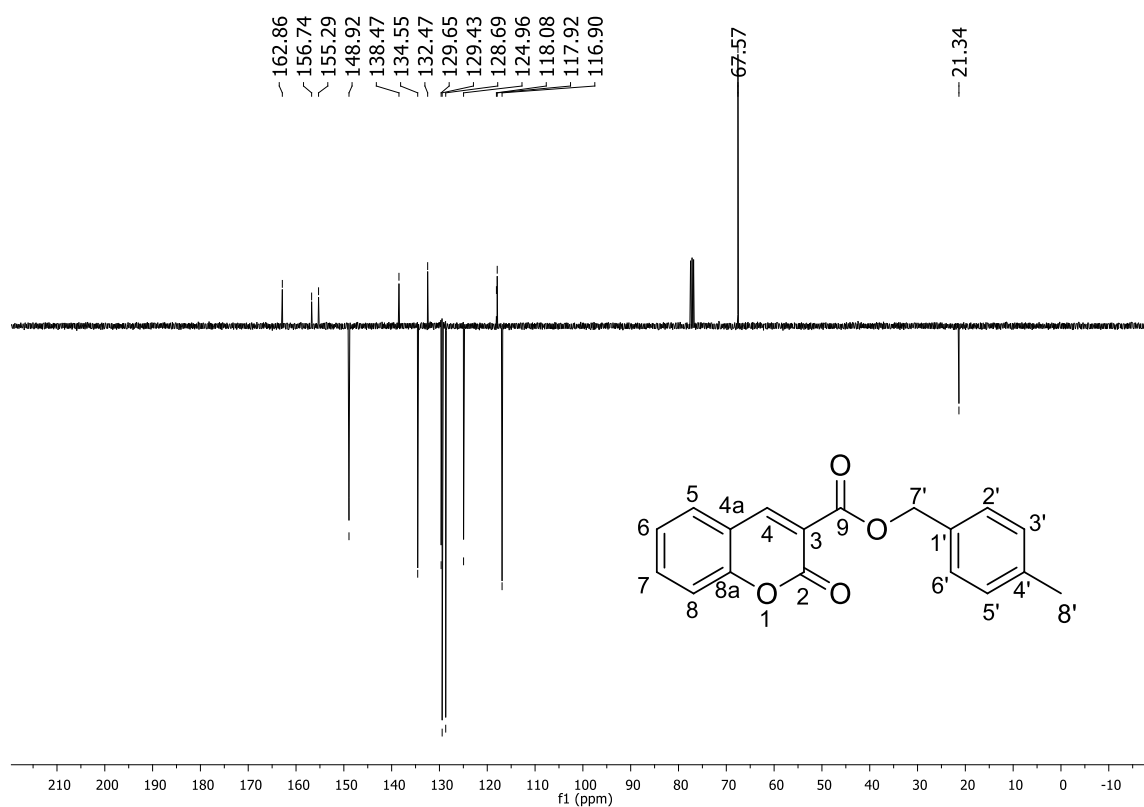


Spectrum S16. HRMS spectrum of compound 11.

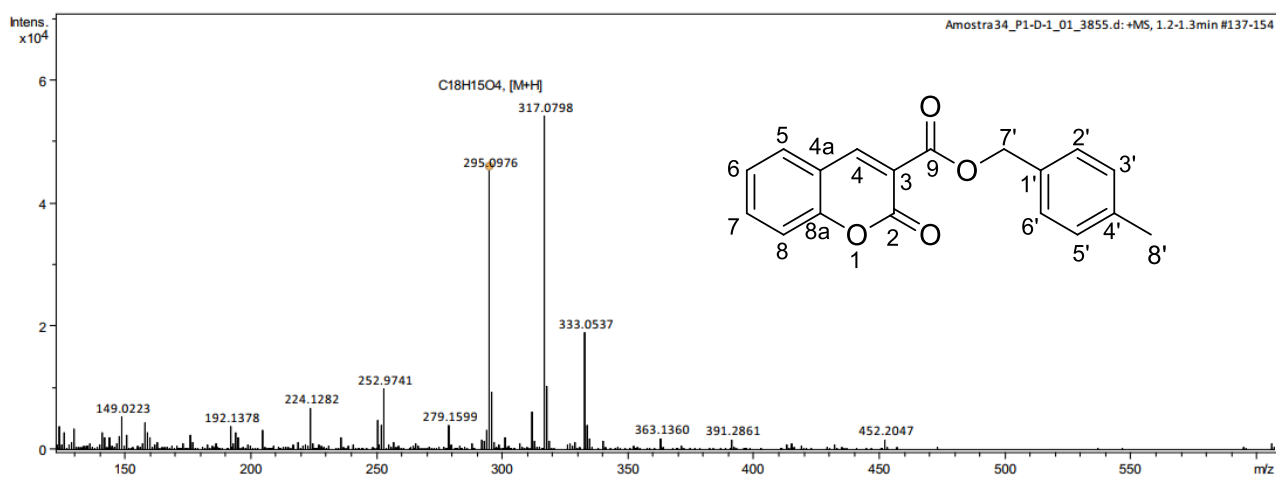


Spectrum S17. Infrared spectrum ν_{\max} (KBr, cm⁻¹) of compound **12**.

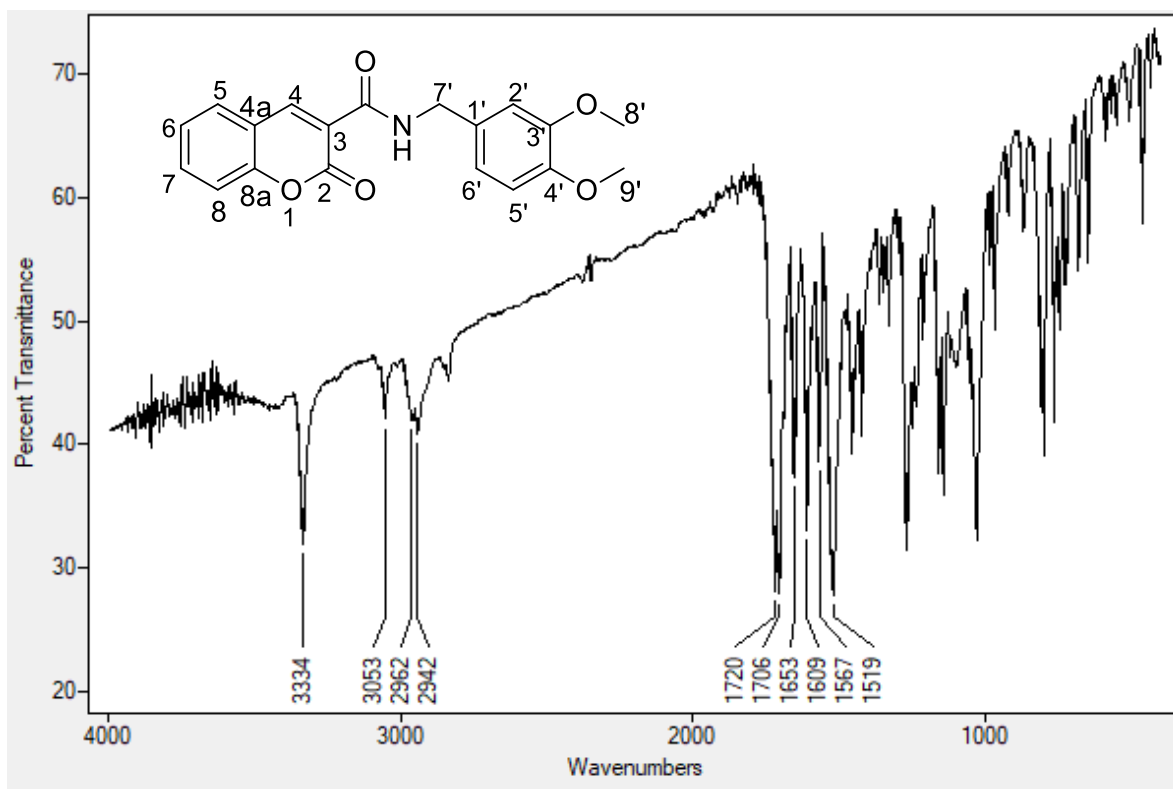




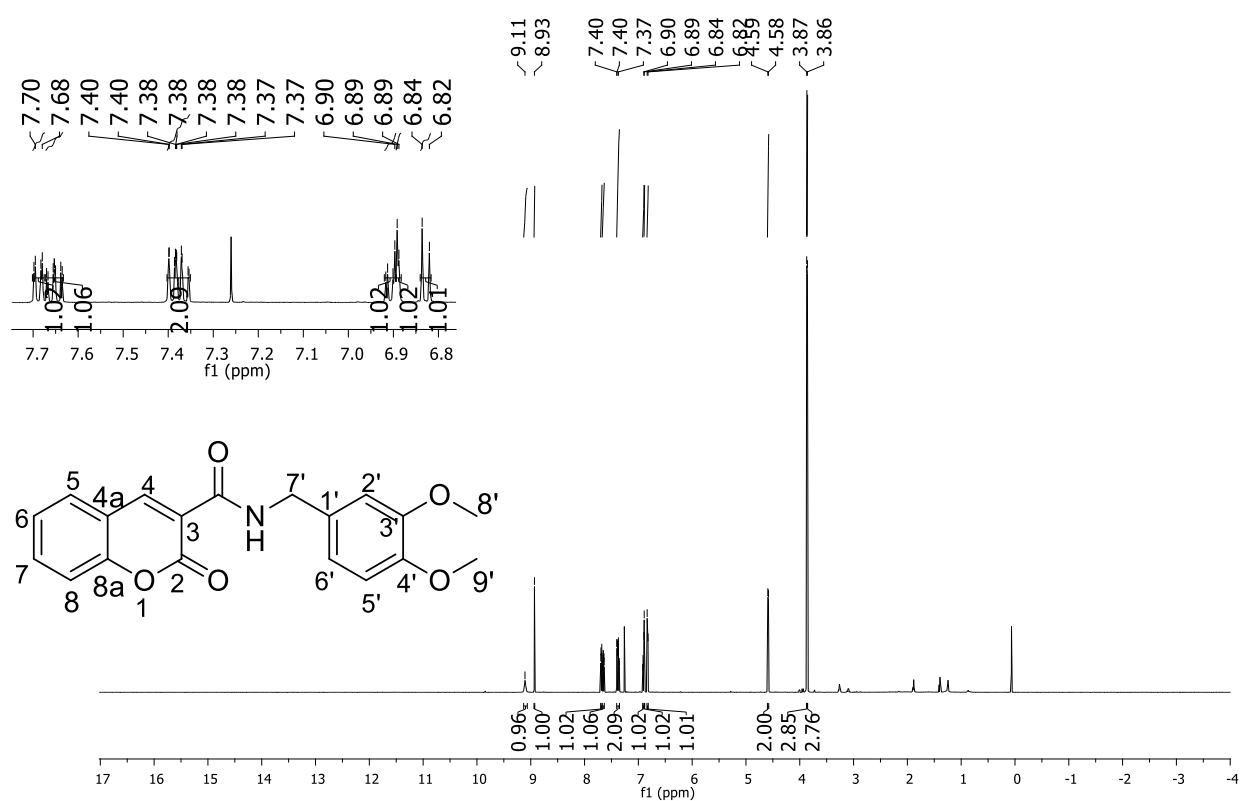
Spectrum S19. ¹³C NMR spectrum (125 MHz, CDCl₃) of compound **12**.



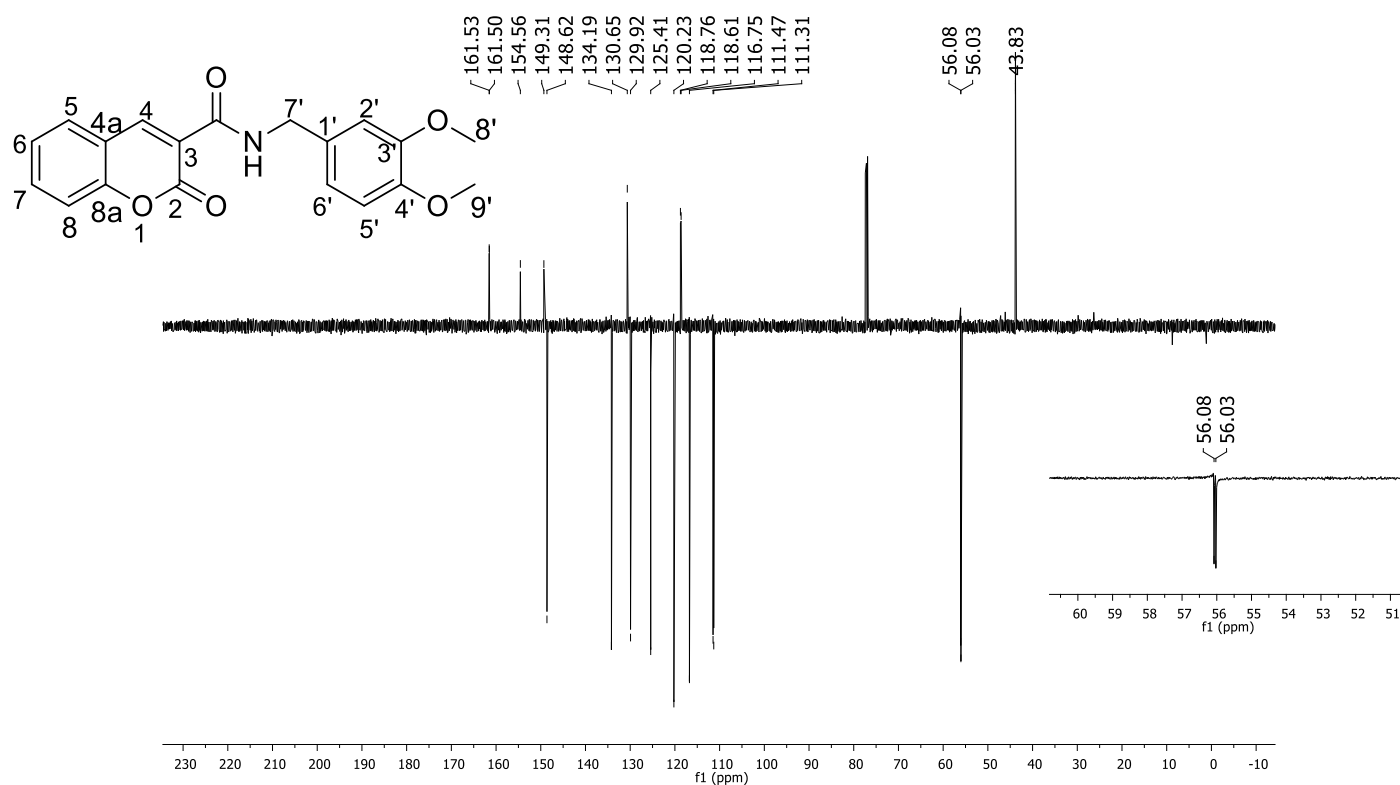
Spectrum S20. HRMS spectrum of compound **12**.



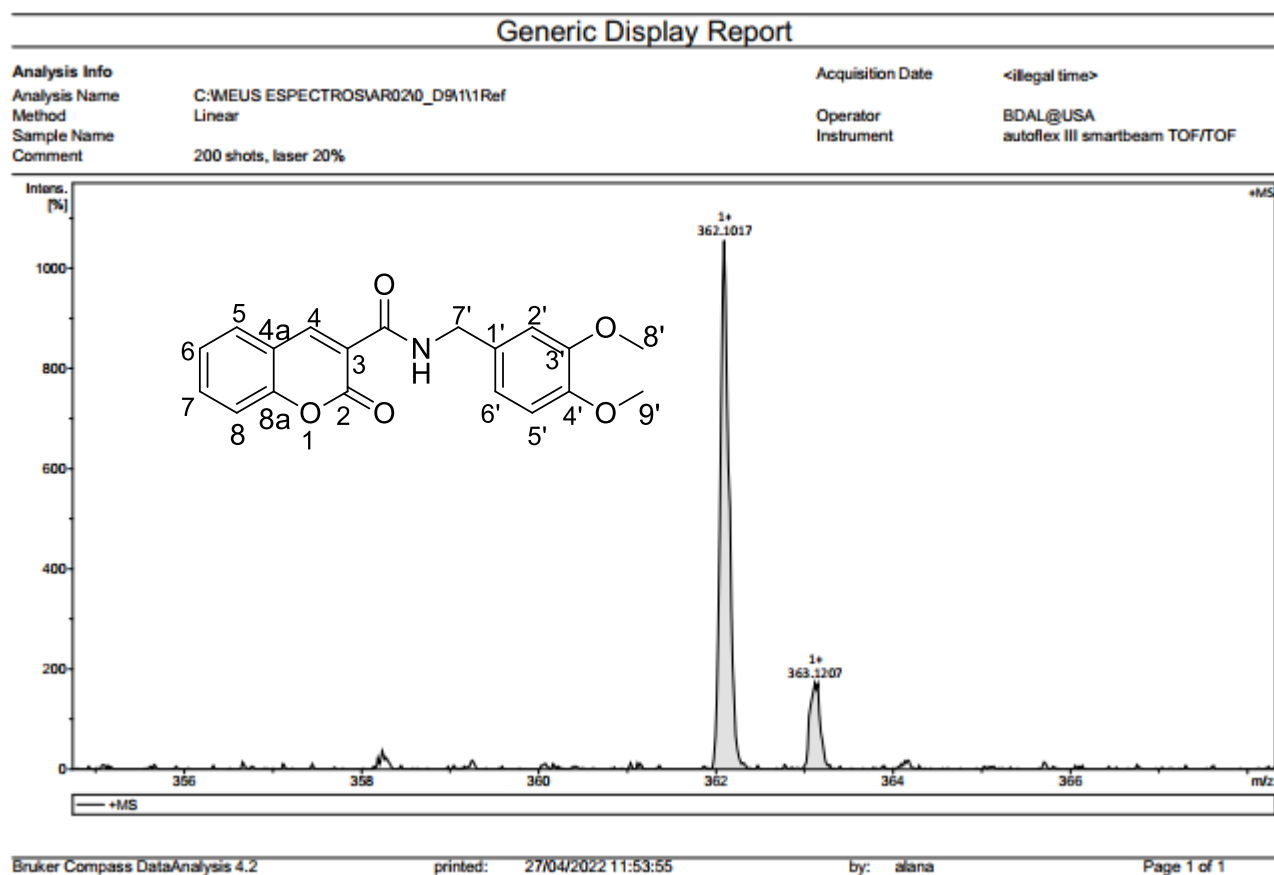
Spectrum S21. Infrared spectrum ν_{\max} (KBr, cm^{-1}) of compound 16.



Spectrum S22. ^1H NMR spectrum (500 MHz, CDCl_3) of compound 16.



Spectrum S23. ¹³C NMR spectrum (125 MHz, CDCl₃) of compound 16.



Spectrum S24. HRMS spectrum of compound 16.