

Synthesis, characterization and optimization of in vitro properties of NIR-fluorescent cyclic α -MSH peptides for melanoma imaging

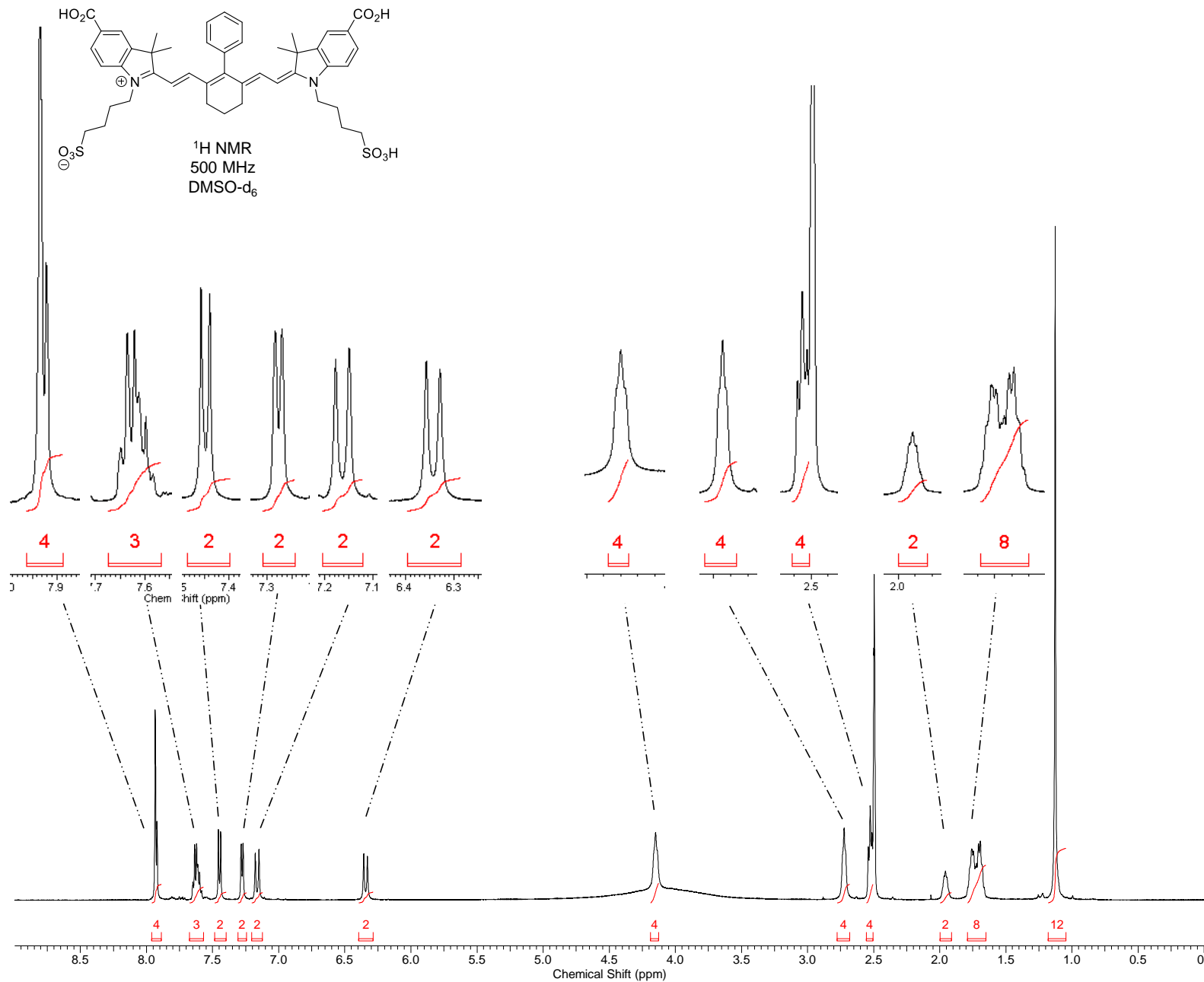
Valeska von Kiedrowski,^{*a} Ralph Hübner,^b Dagmar Kail,^a Xia Cheng,^a Ralf Schirmacher,^c Carmen Wängler^b and Björn Wängler^{*a}

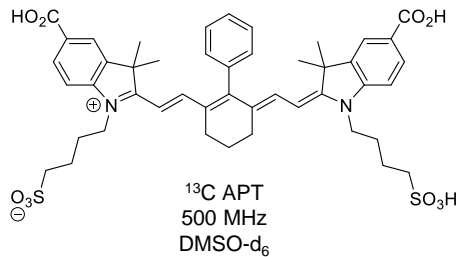
Supporting Information, Part 2

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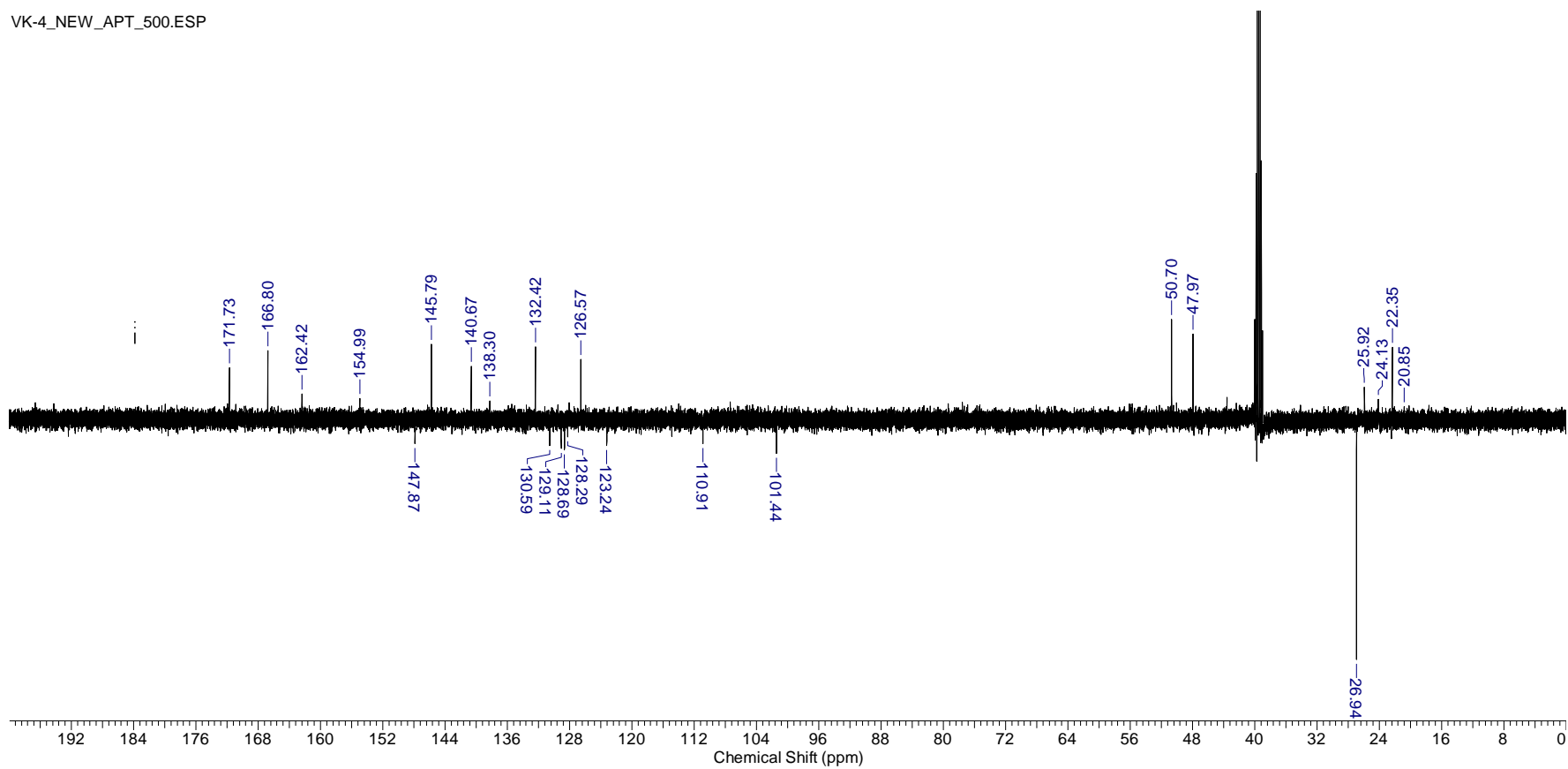
Table of Contents

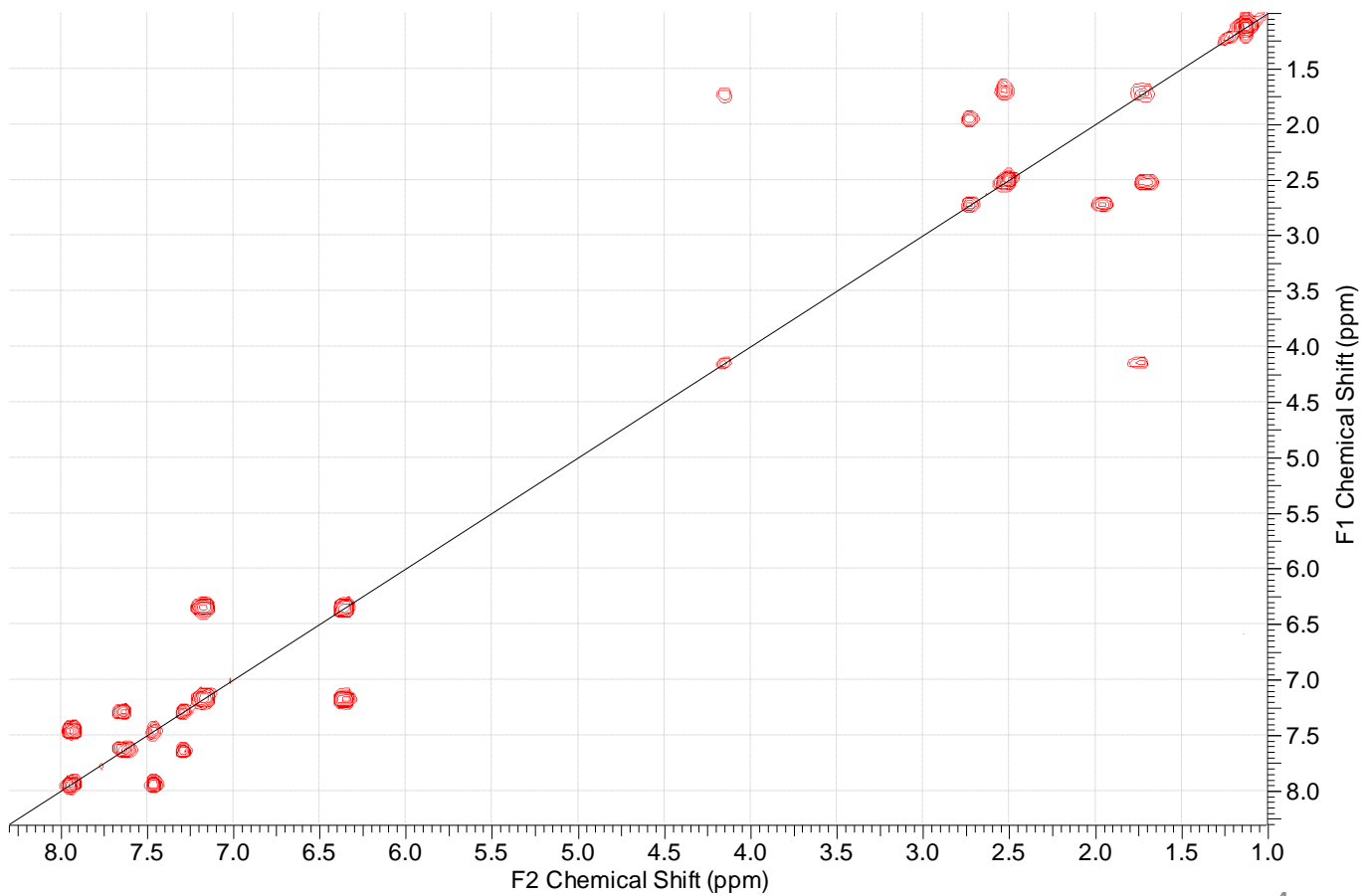
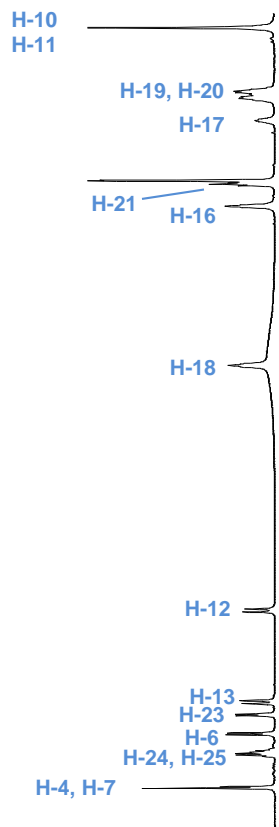
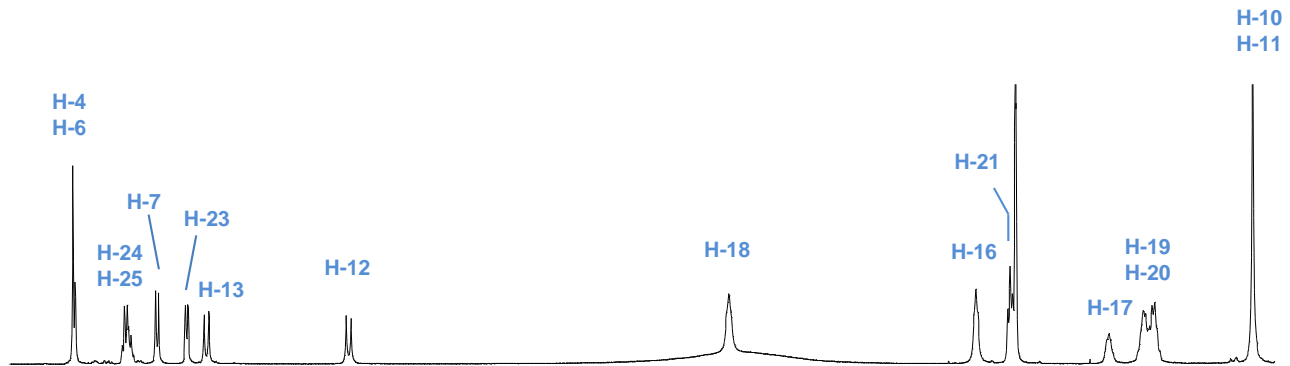
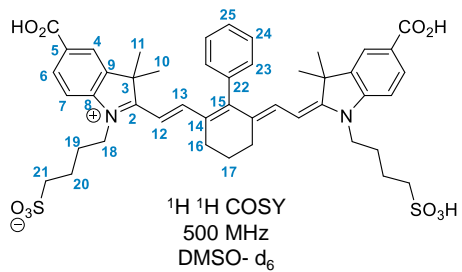
Copies of NMR spectra	2
Absorbance and Emission, Maldi-MS Spectra, HPLC Chromatogramm ESI-MS Spectra	21

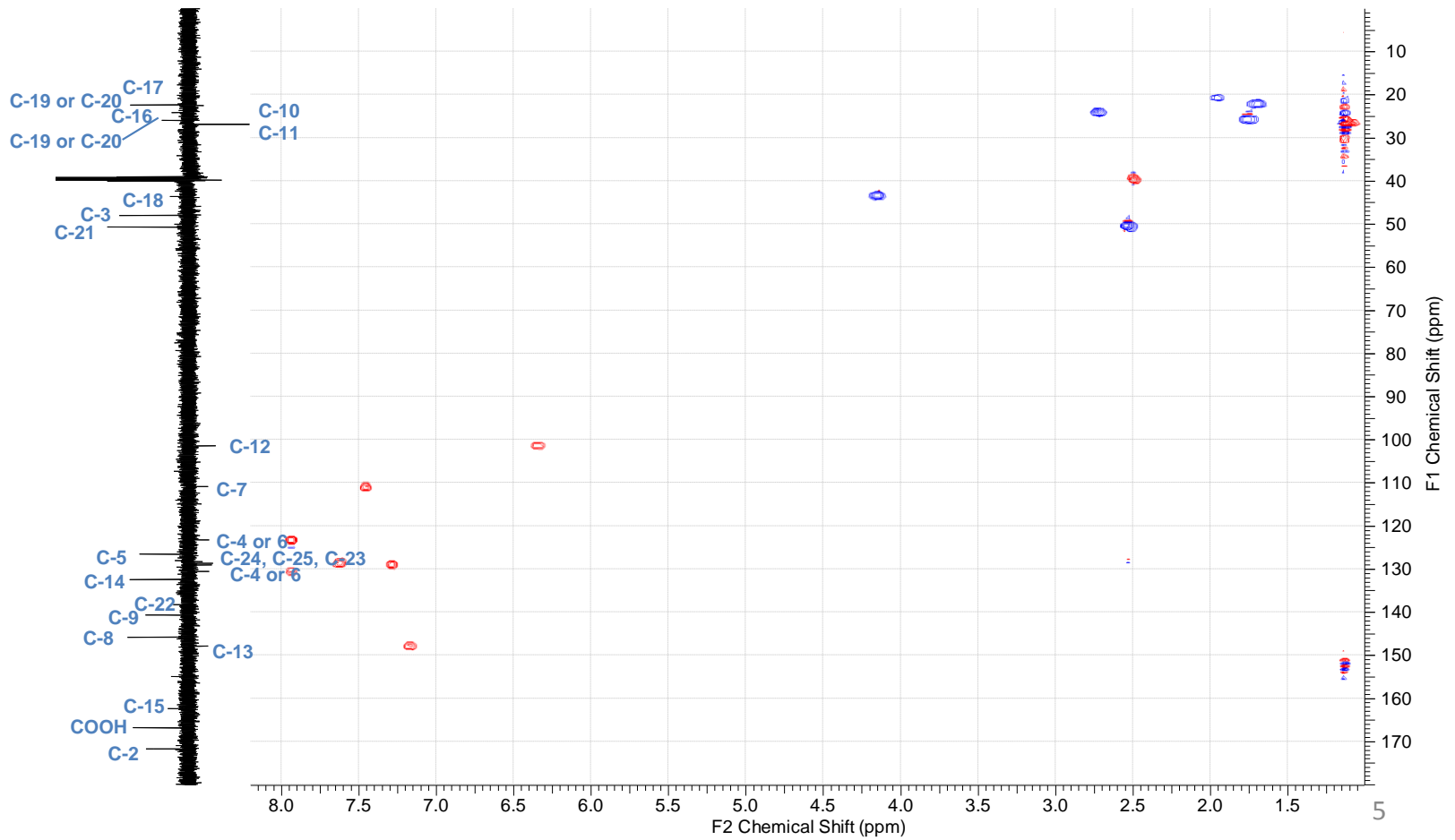
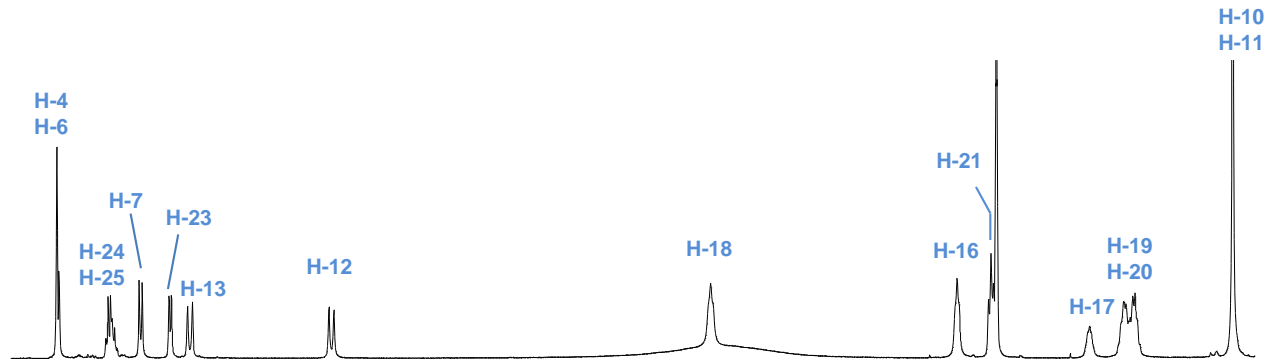
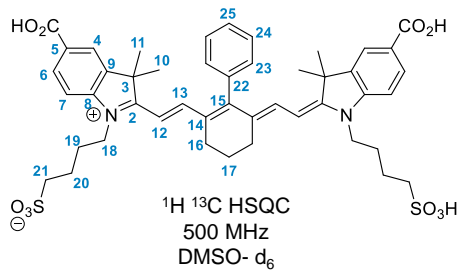


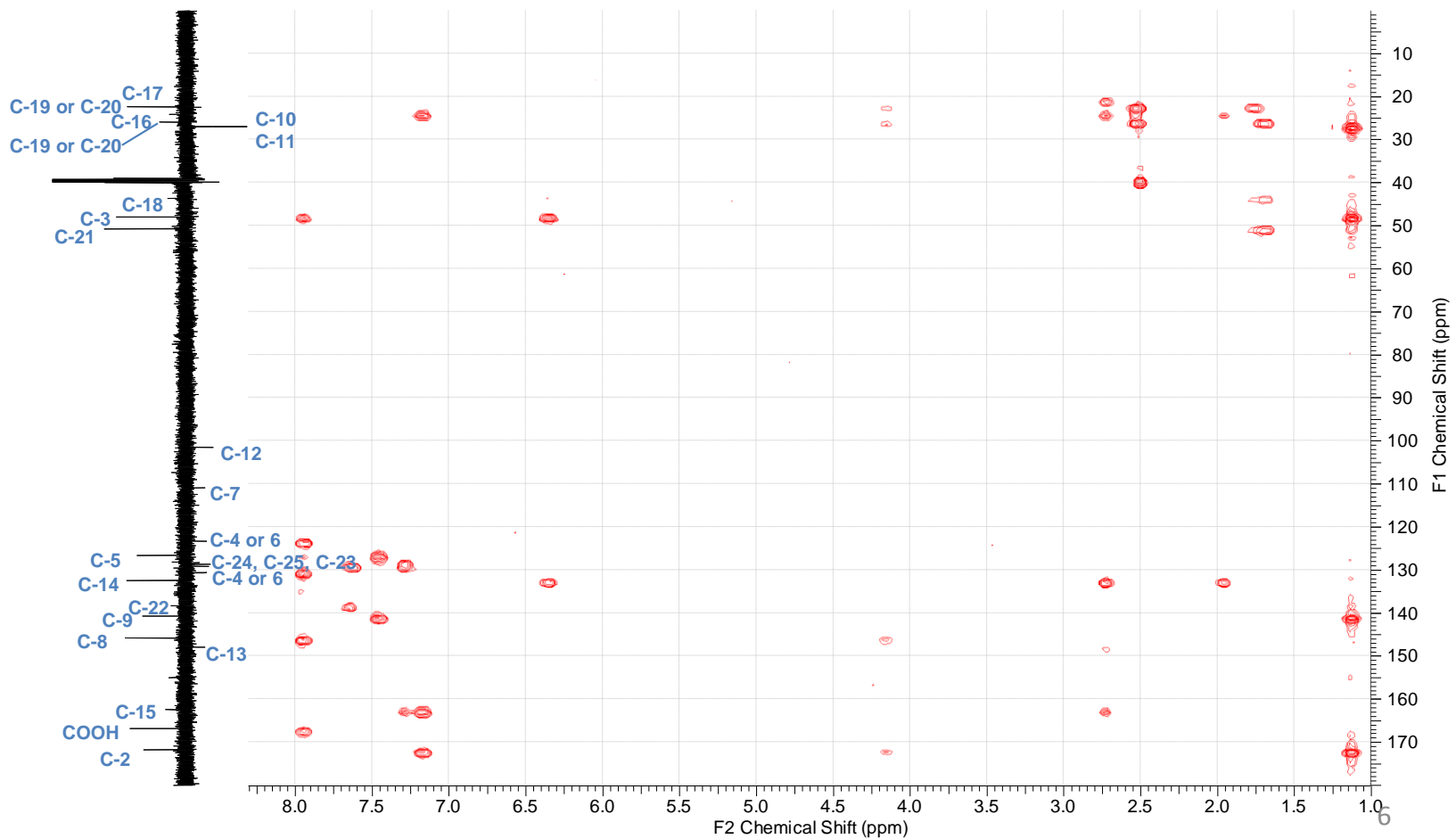
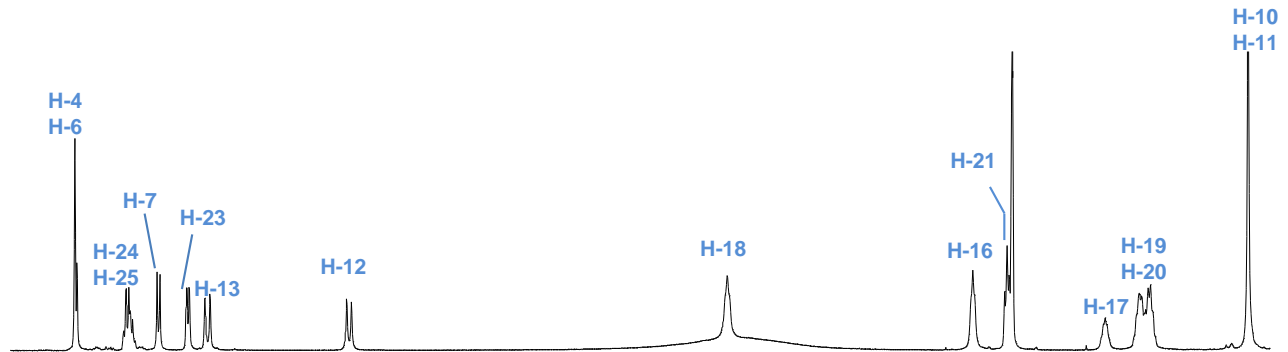
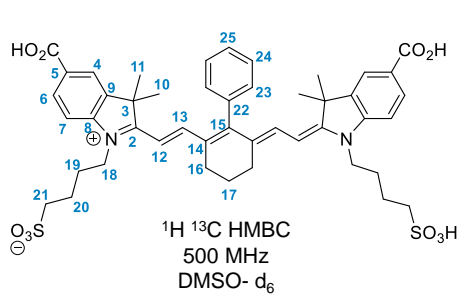


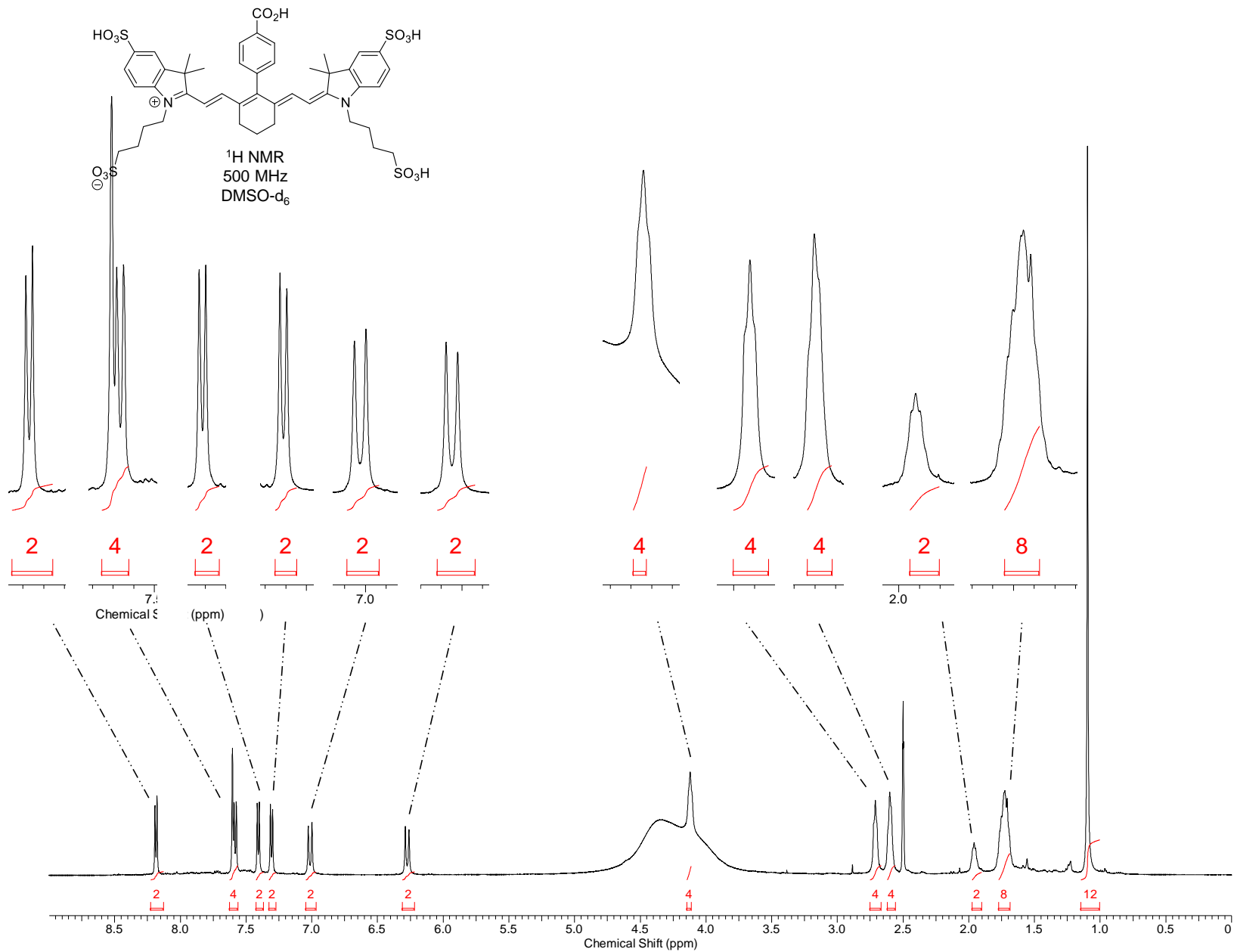
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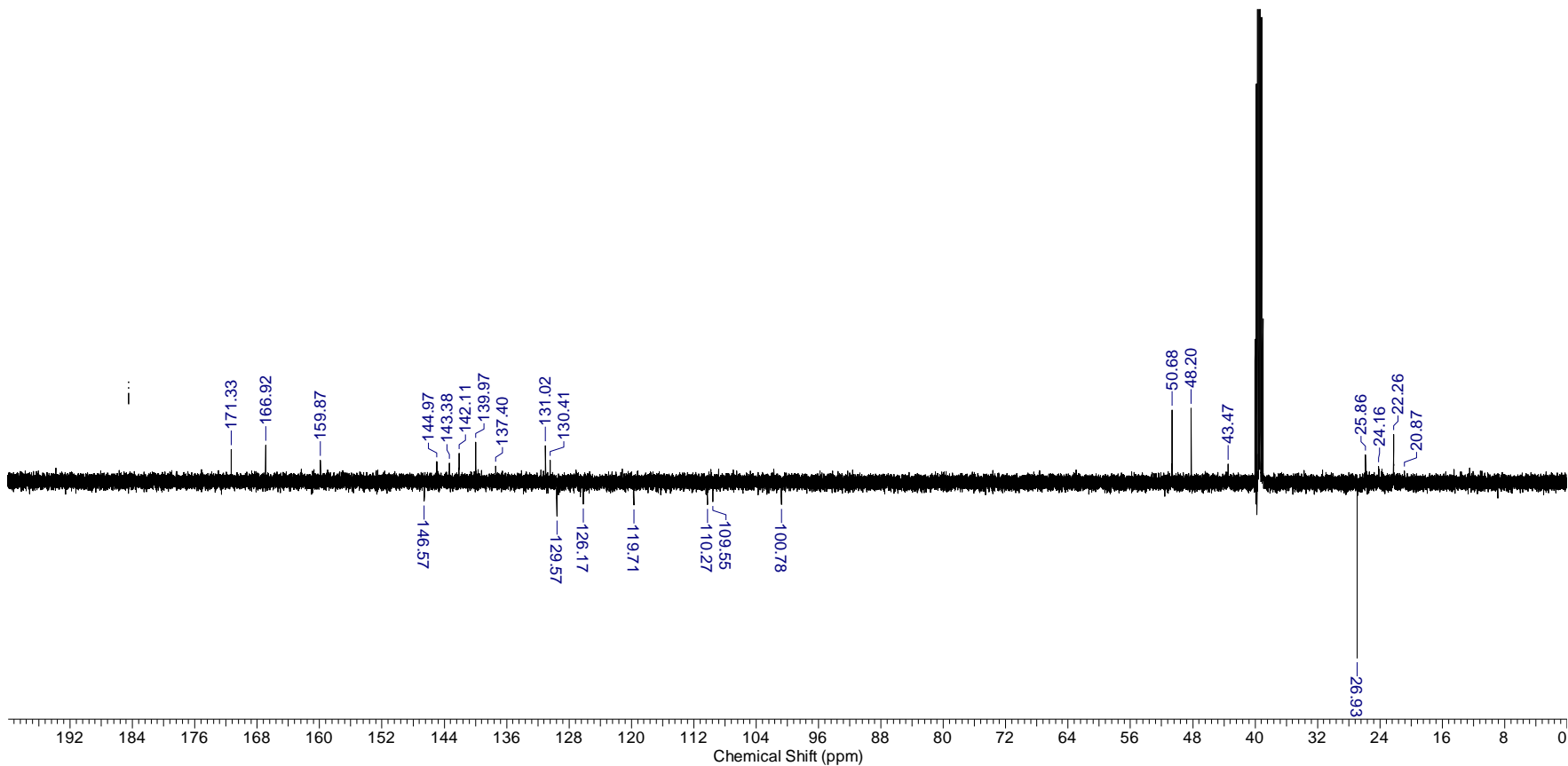
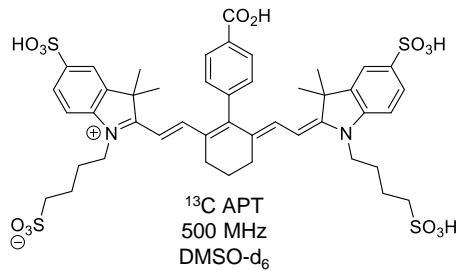


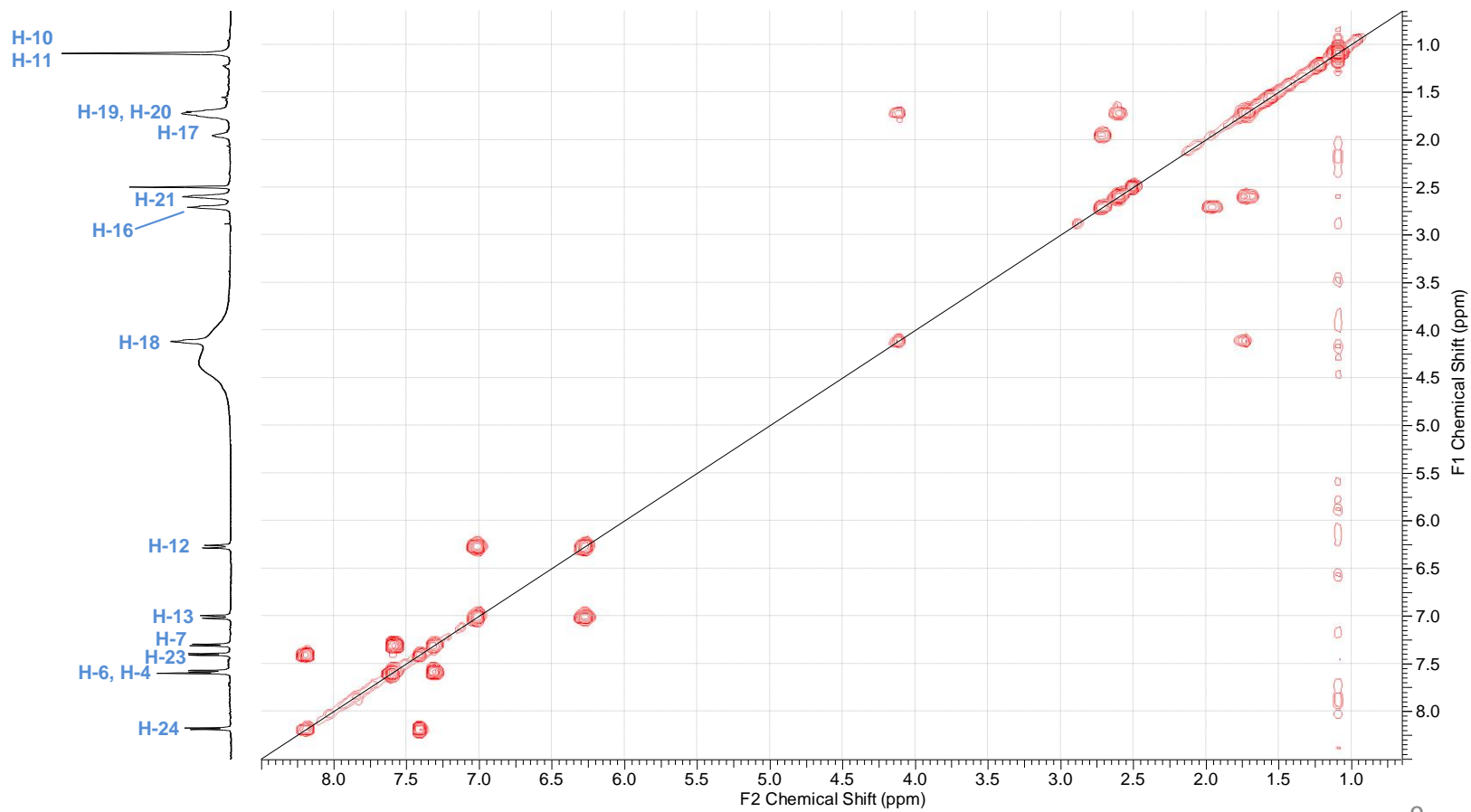
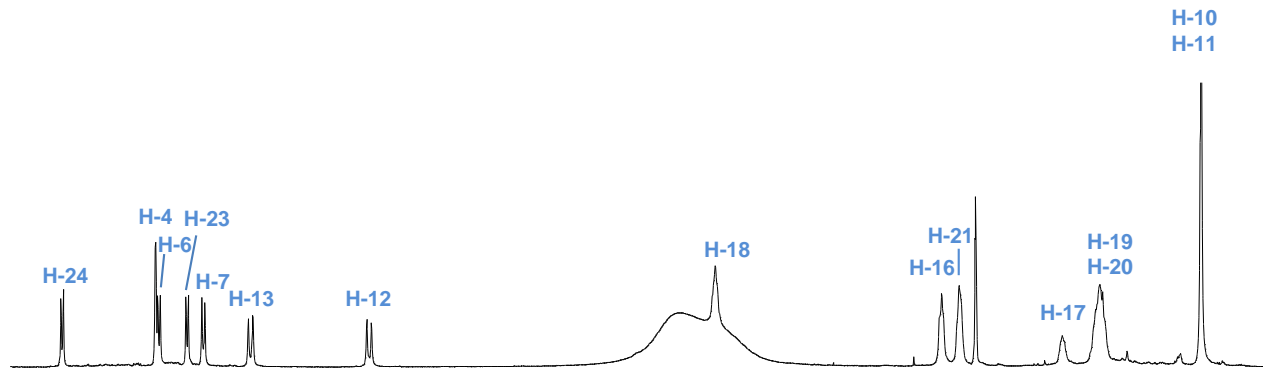
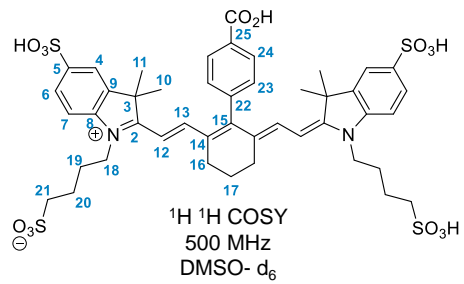


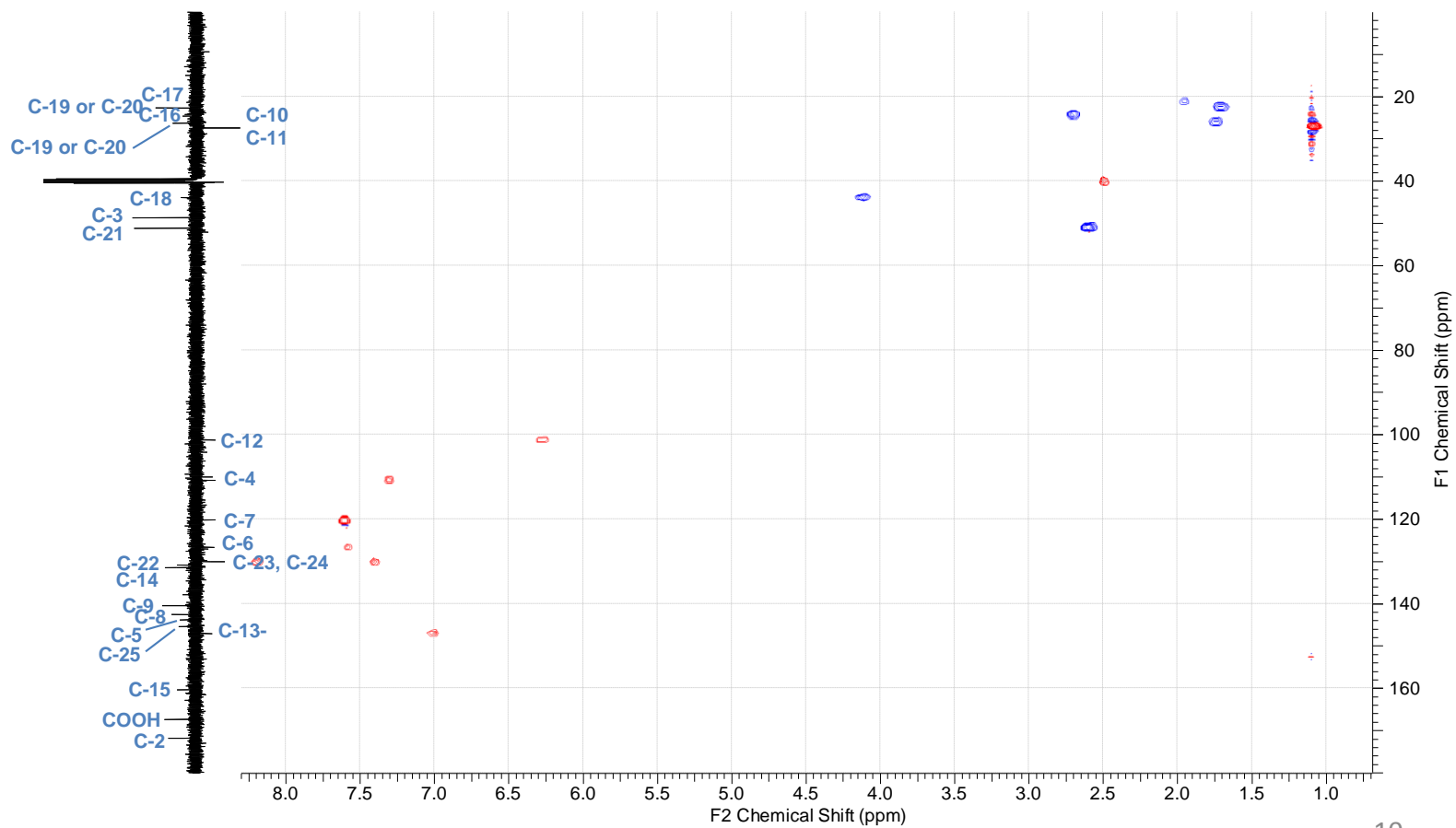
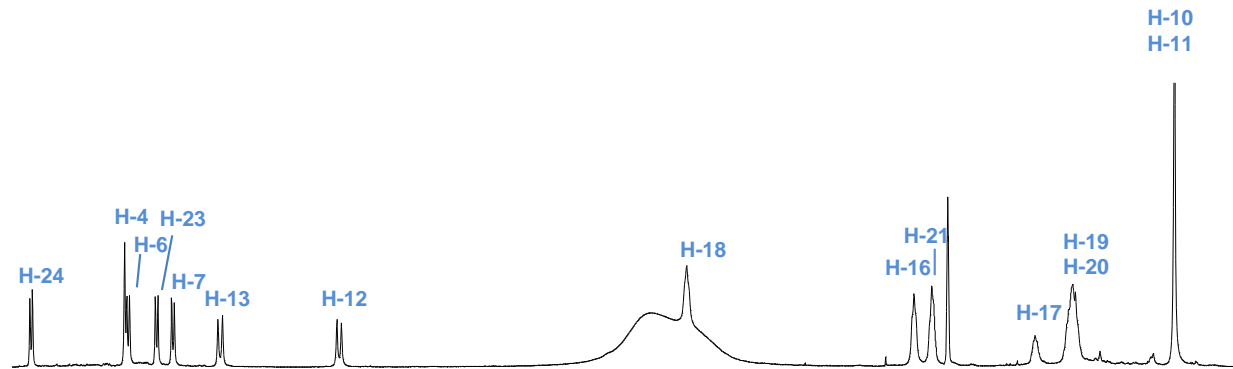
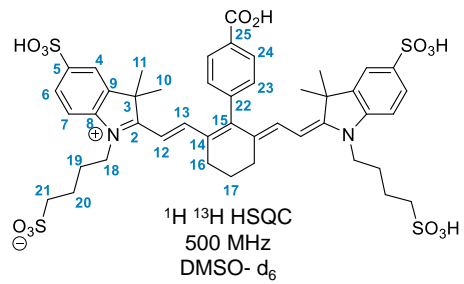


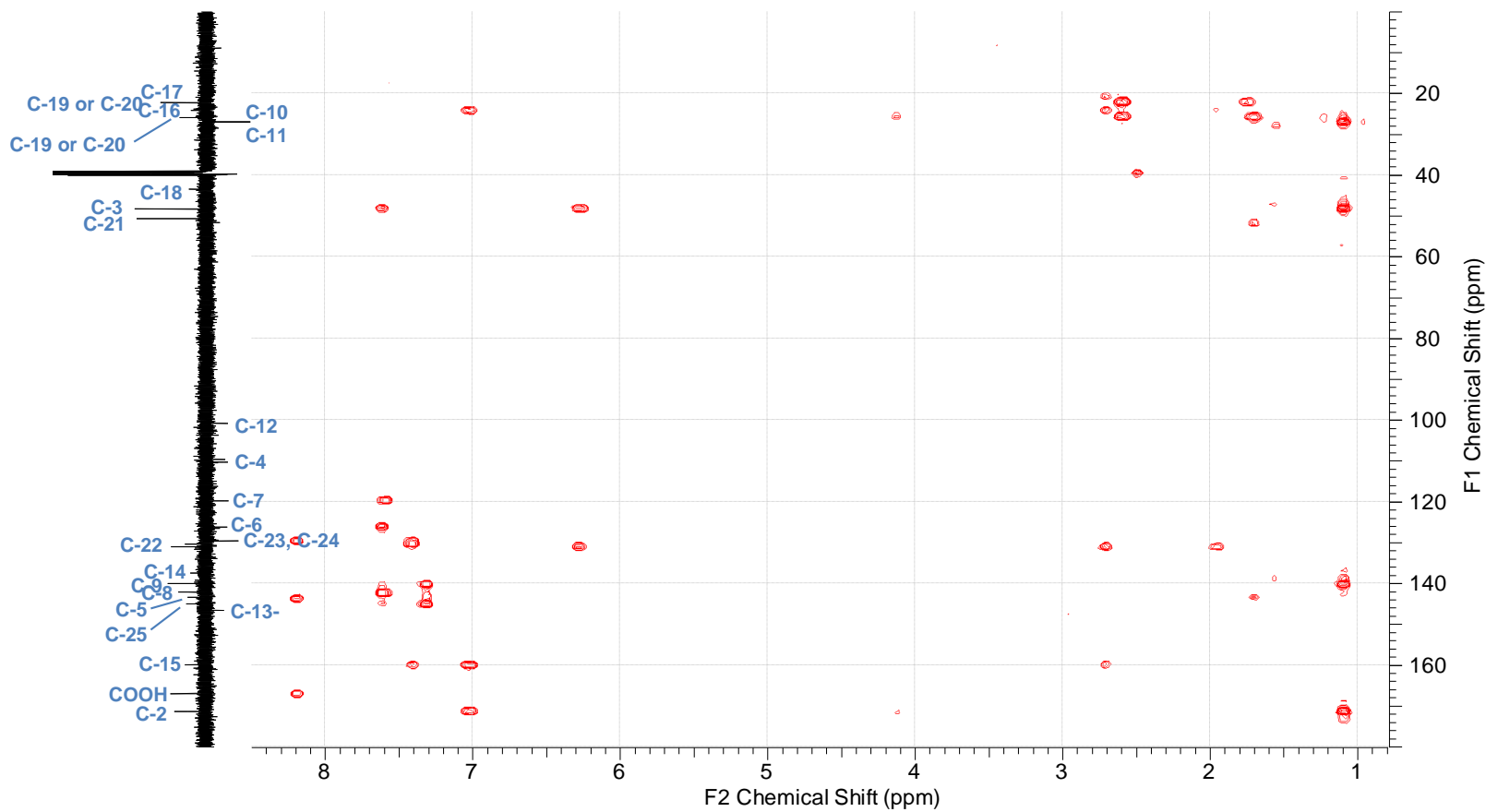
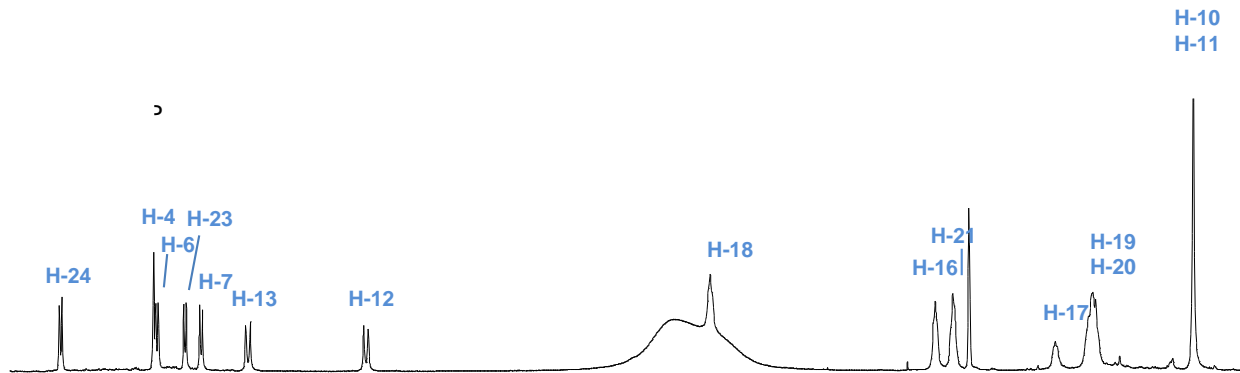
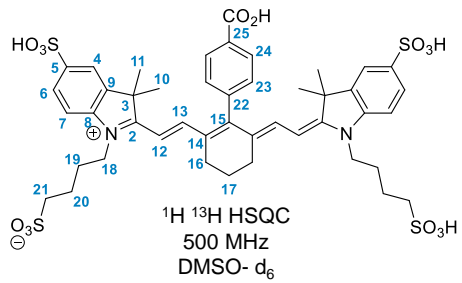


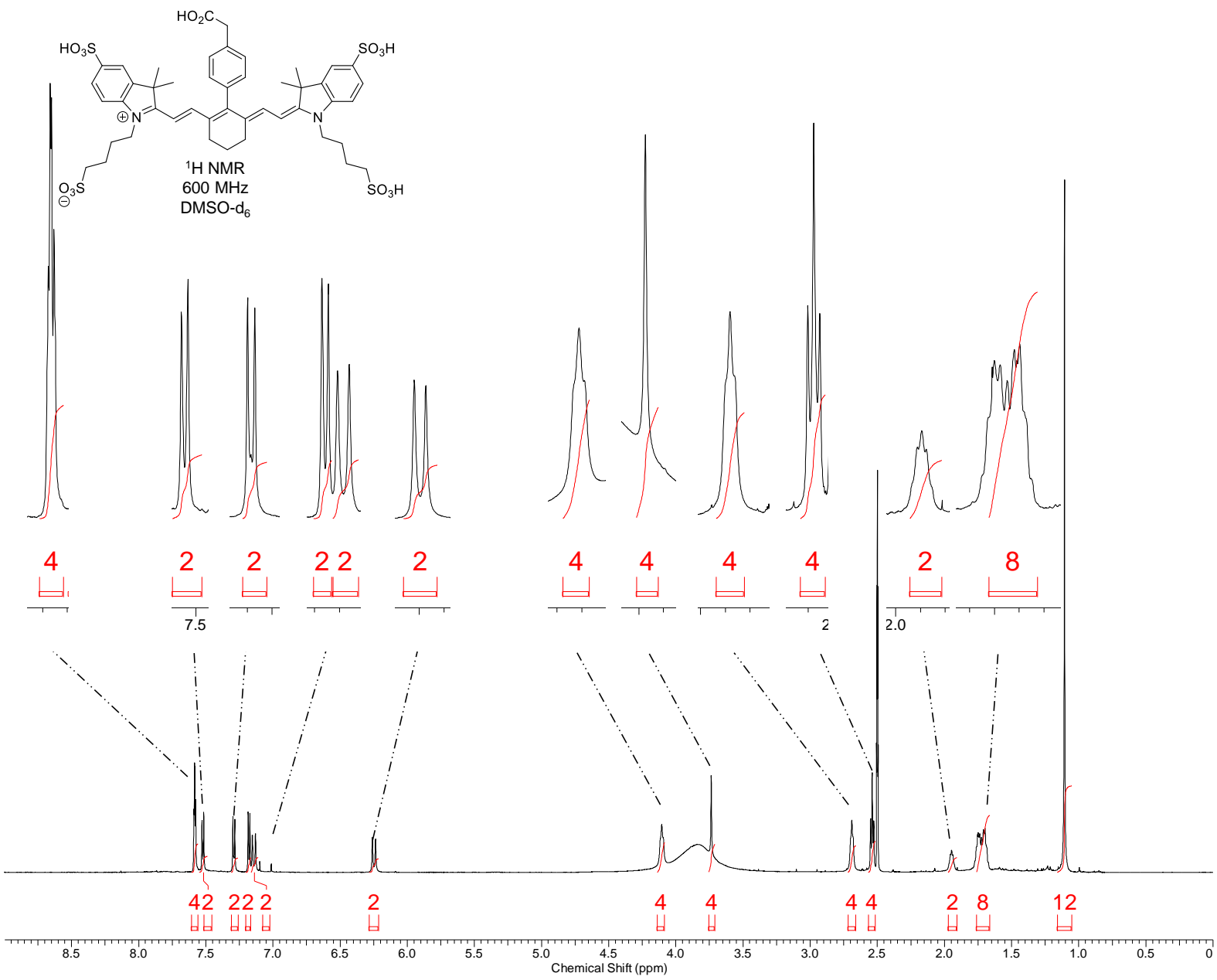


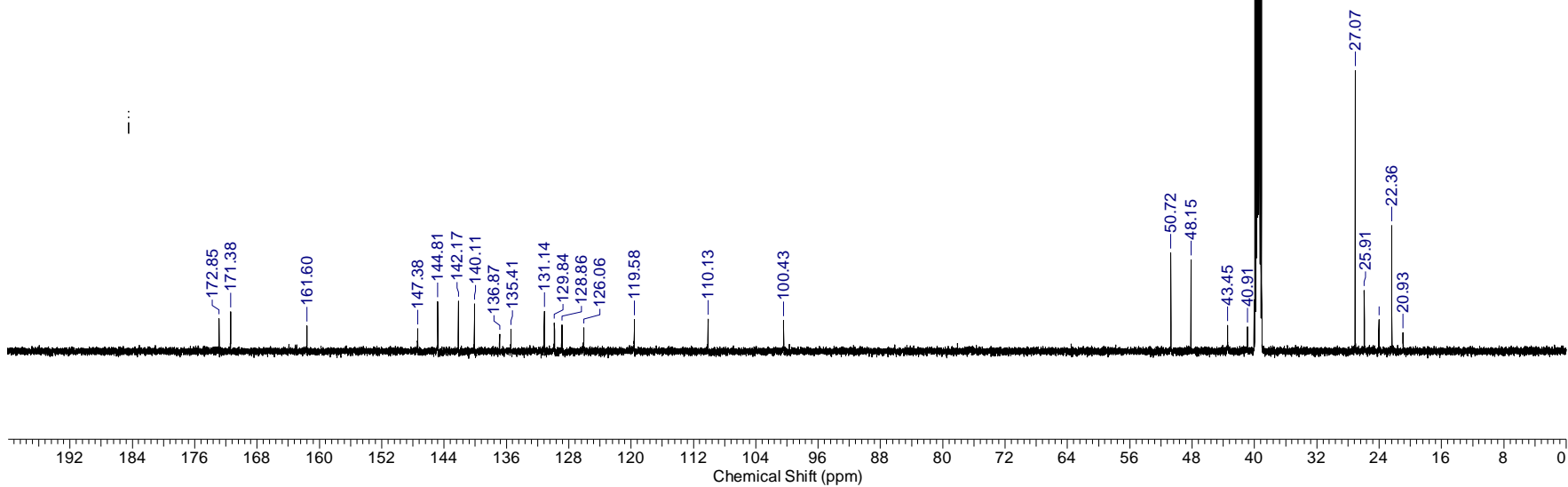
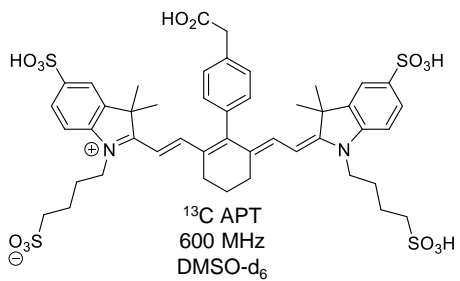


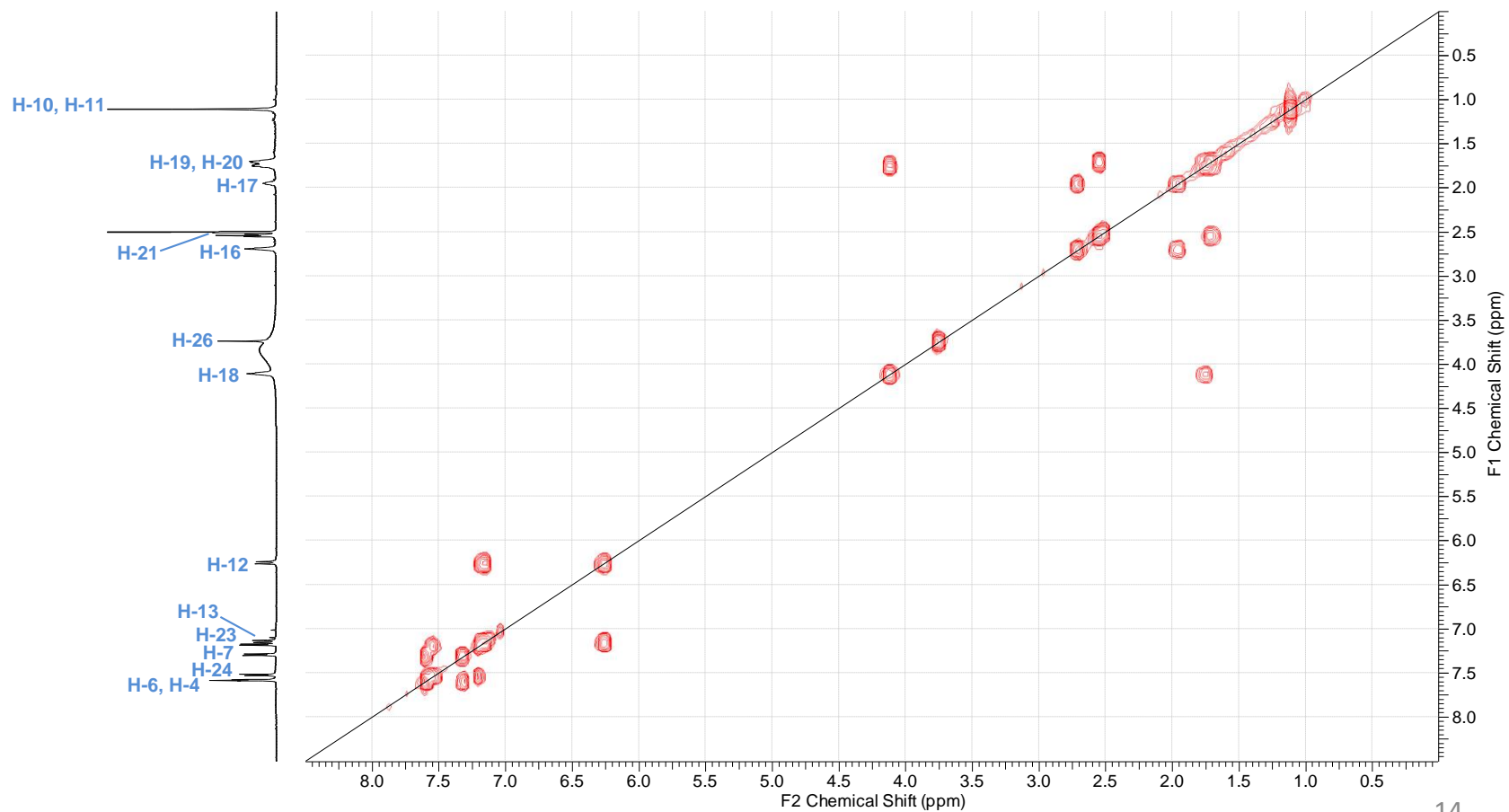
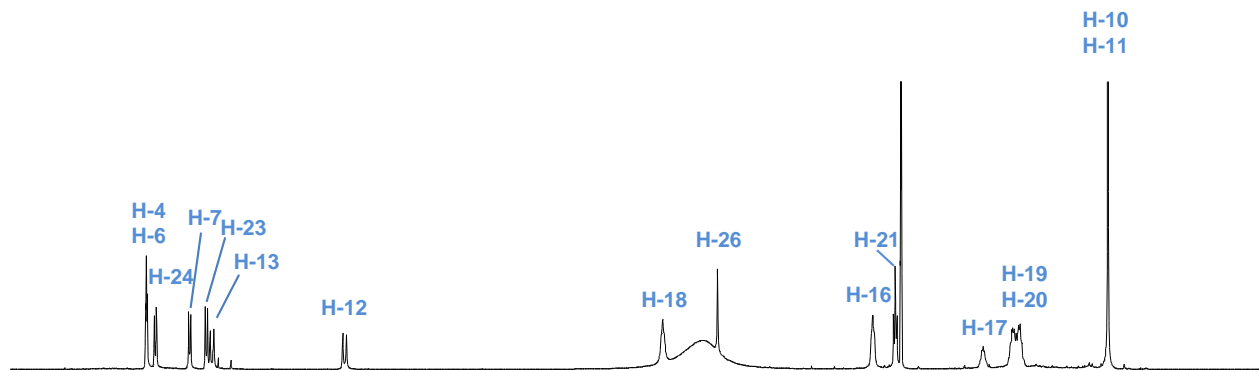
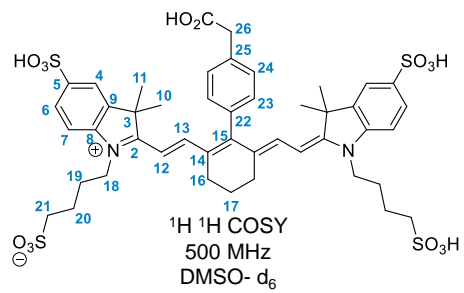


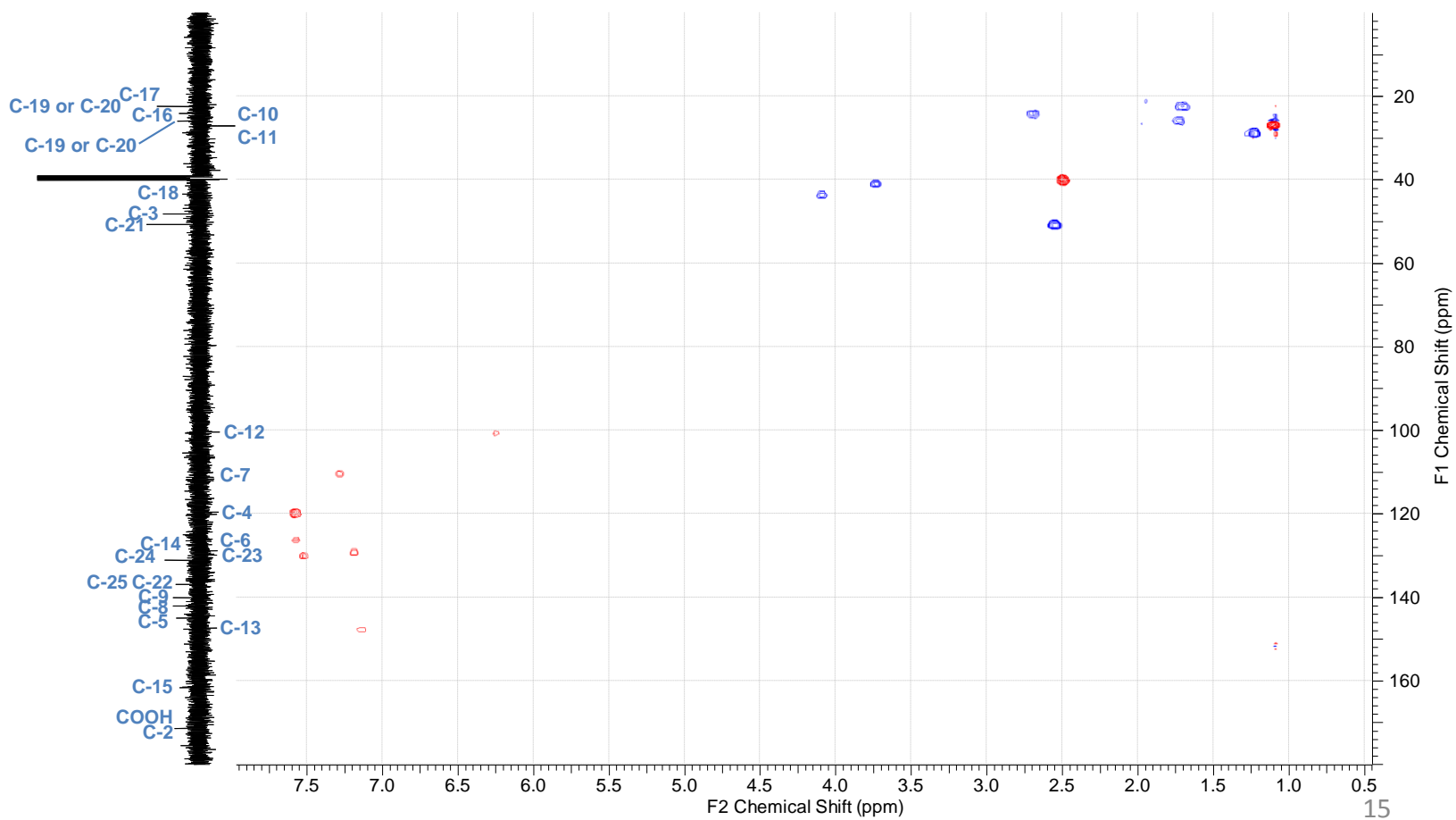
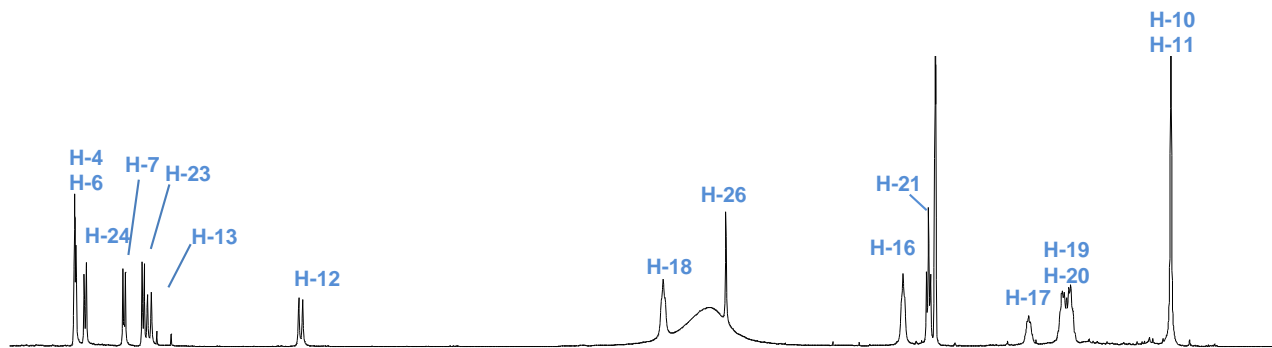
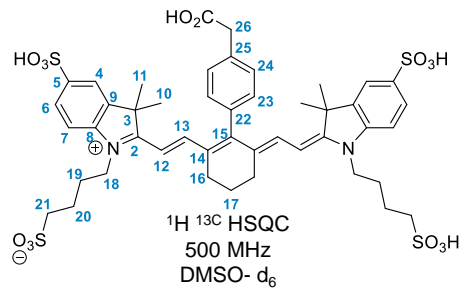


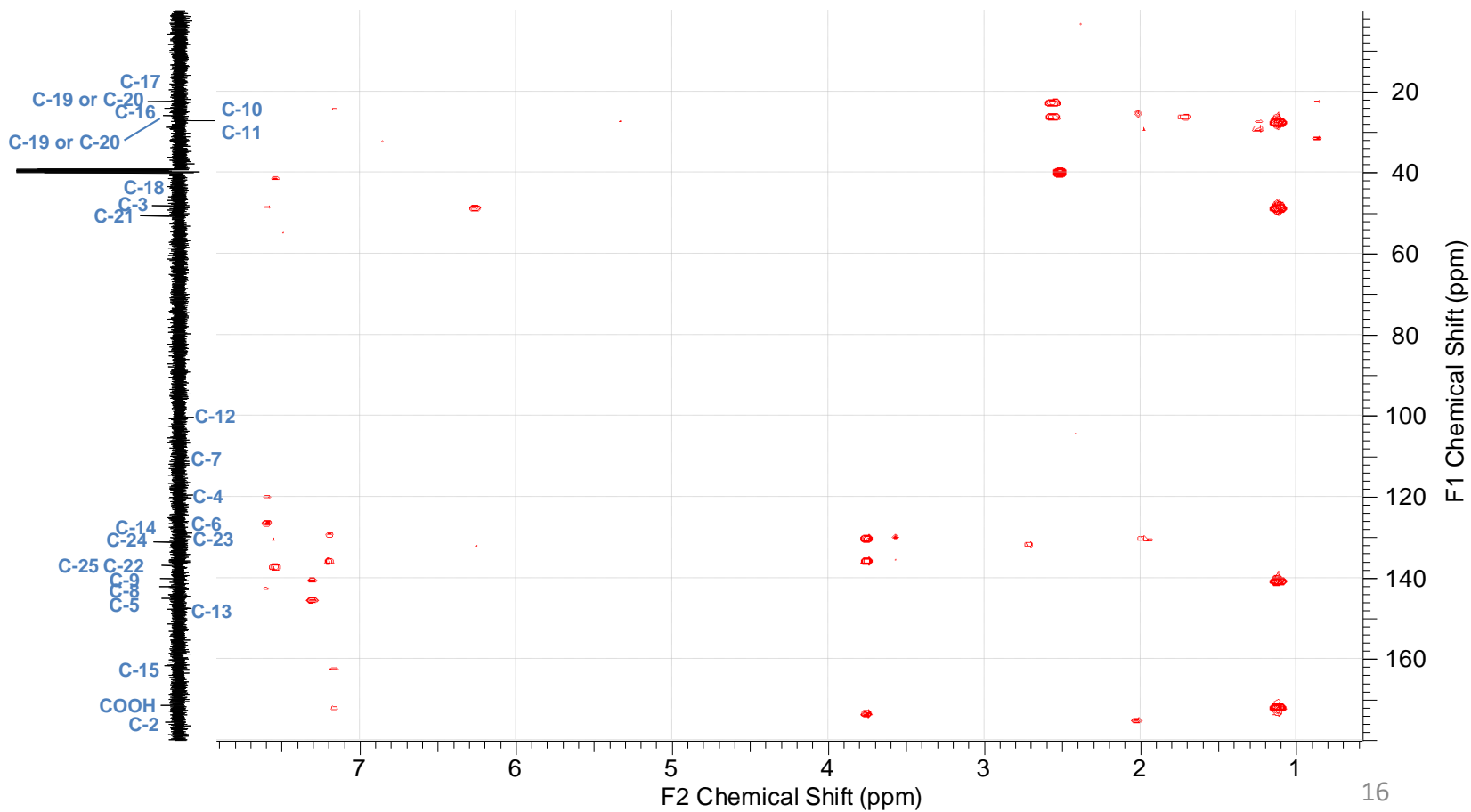
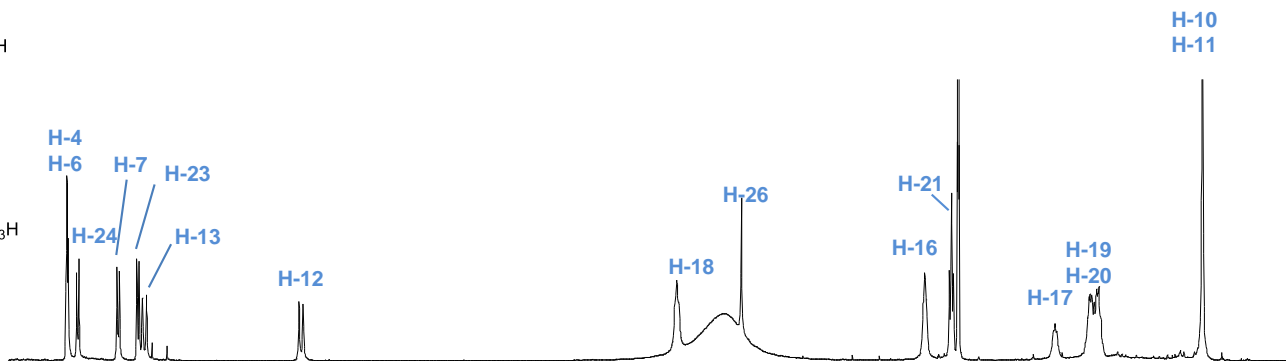
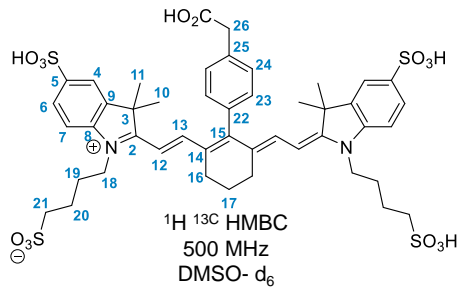


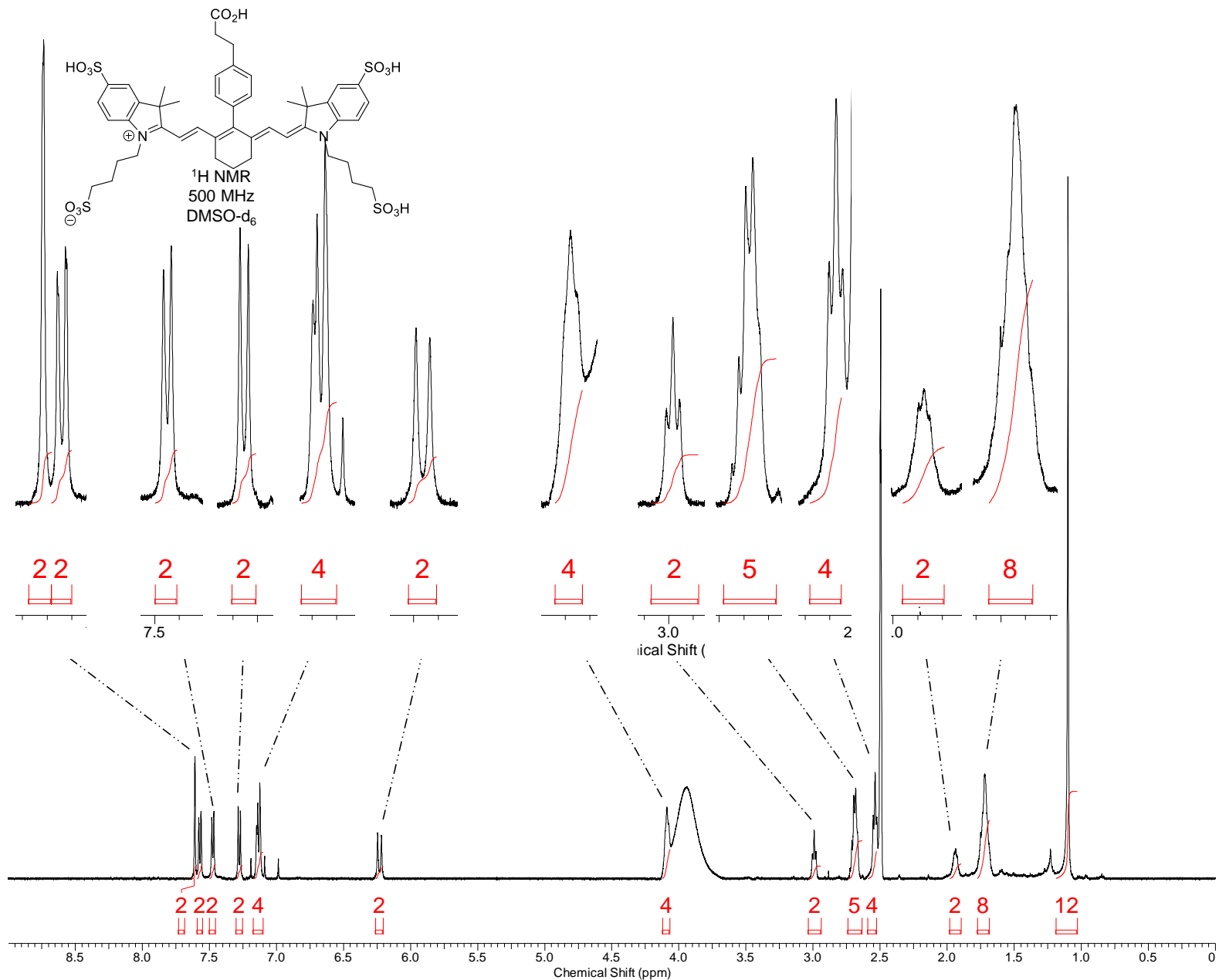


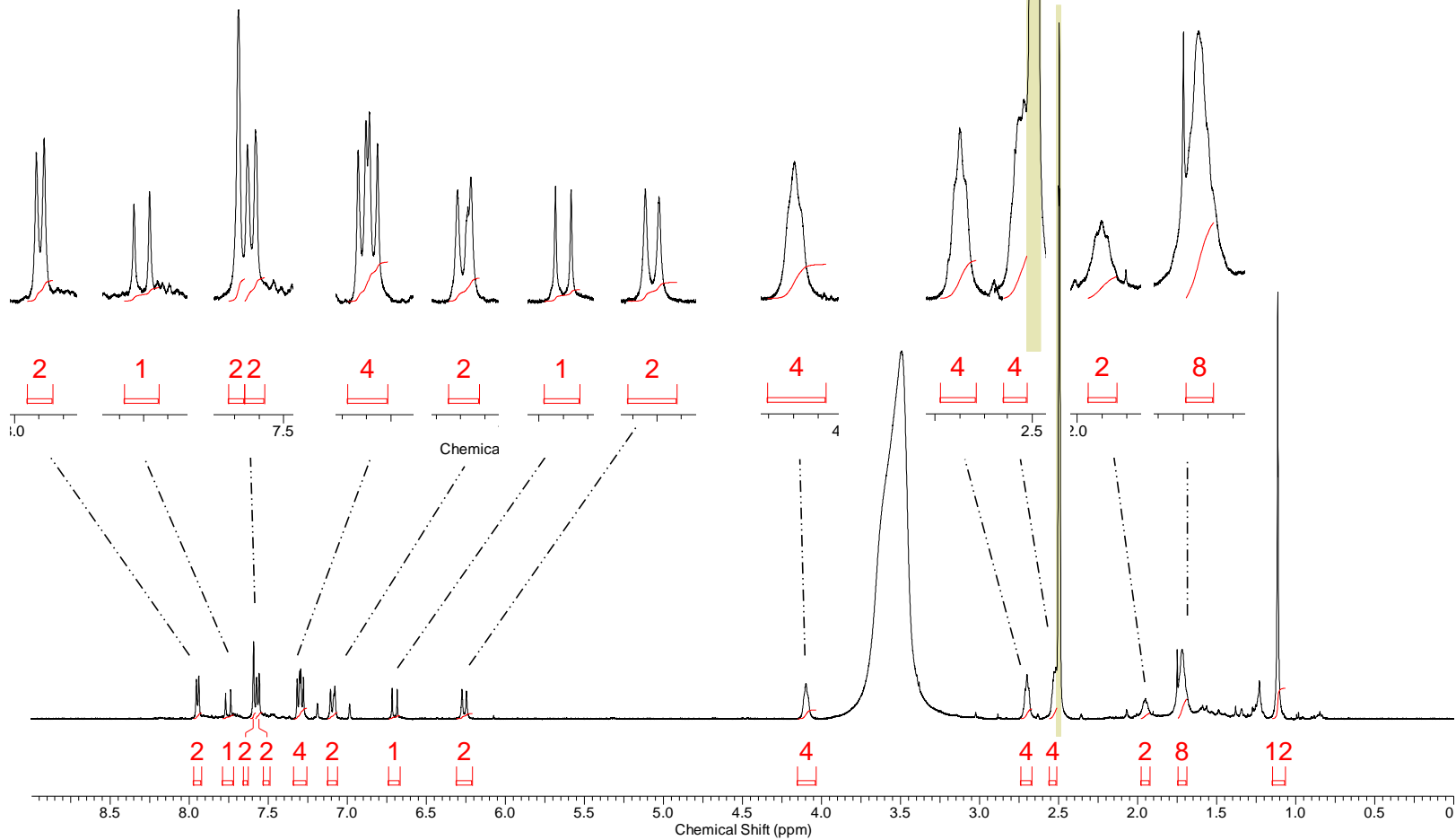
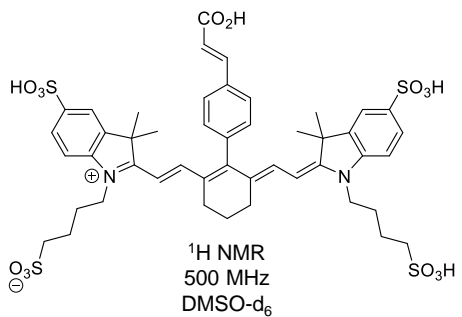


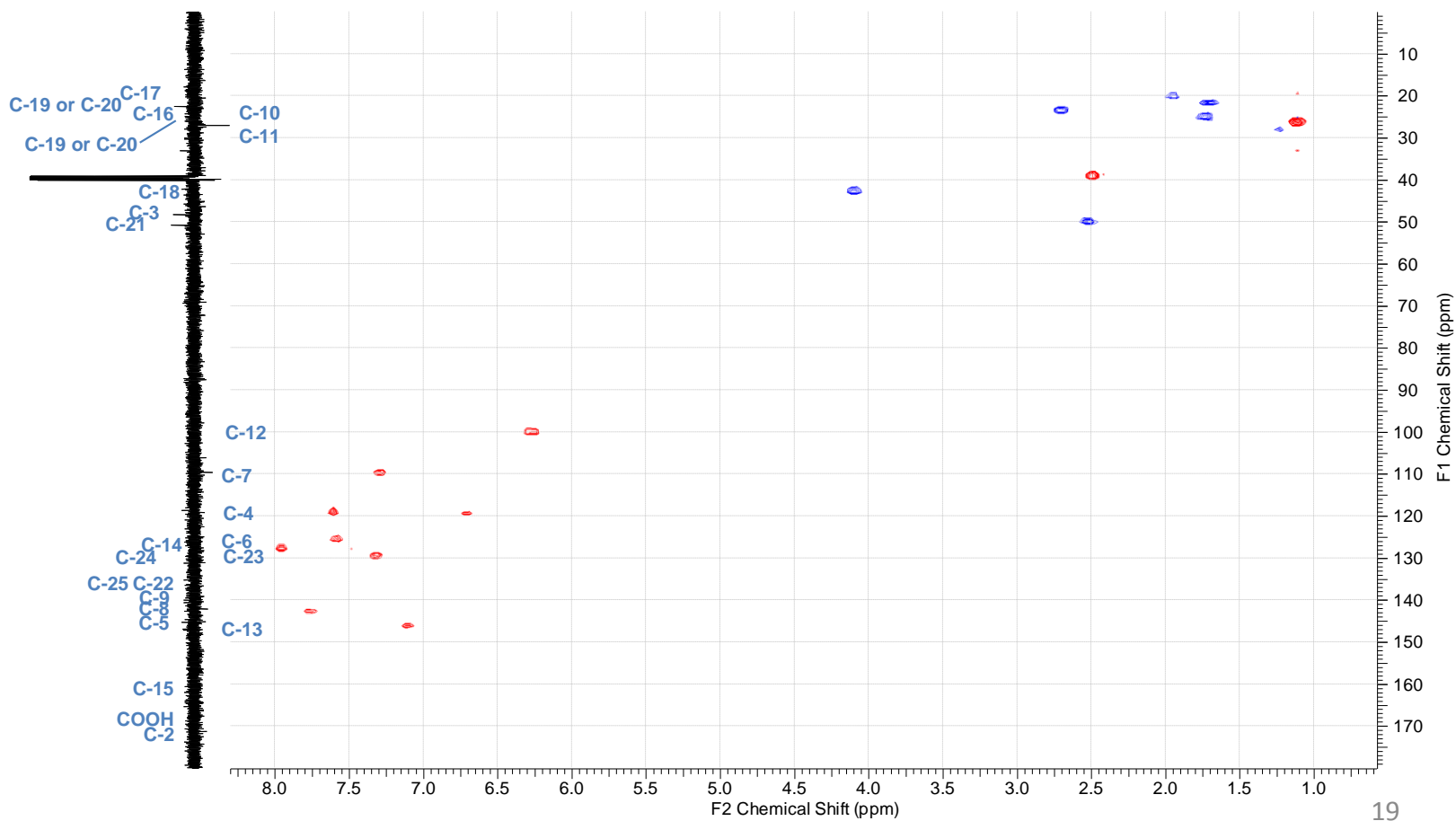
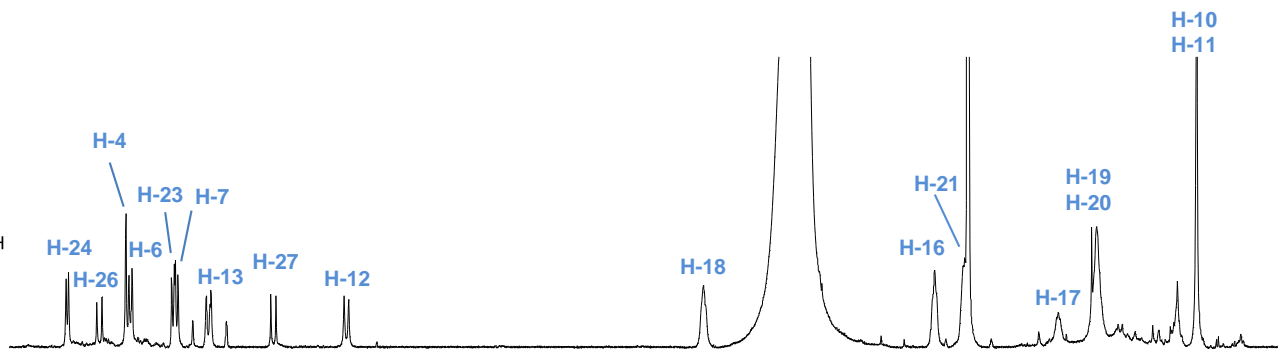
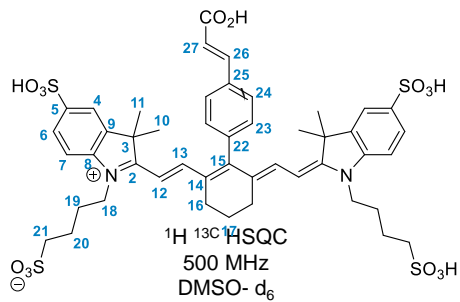


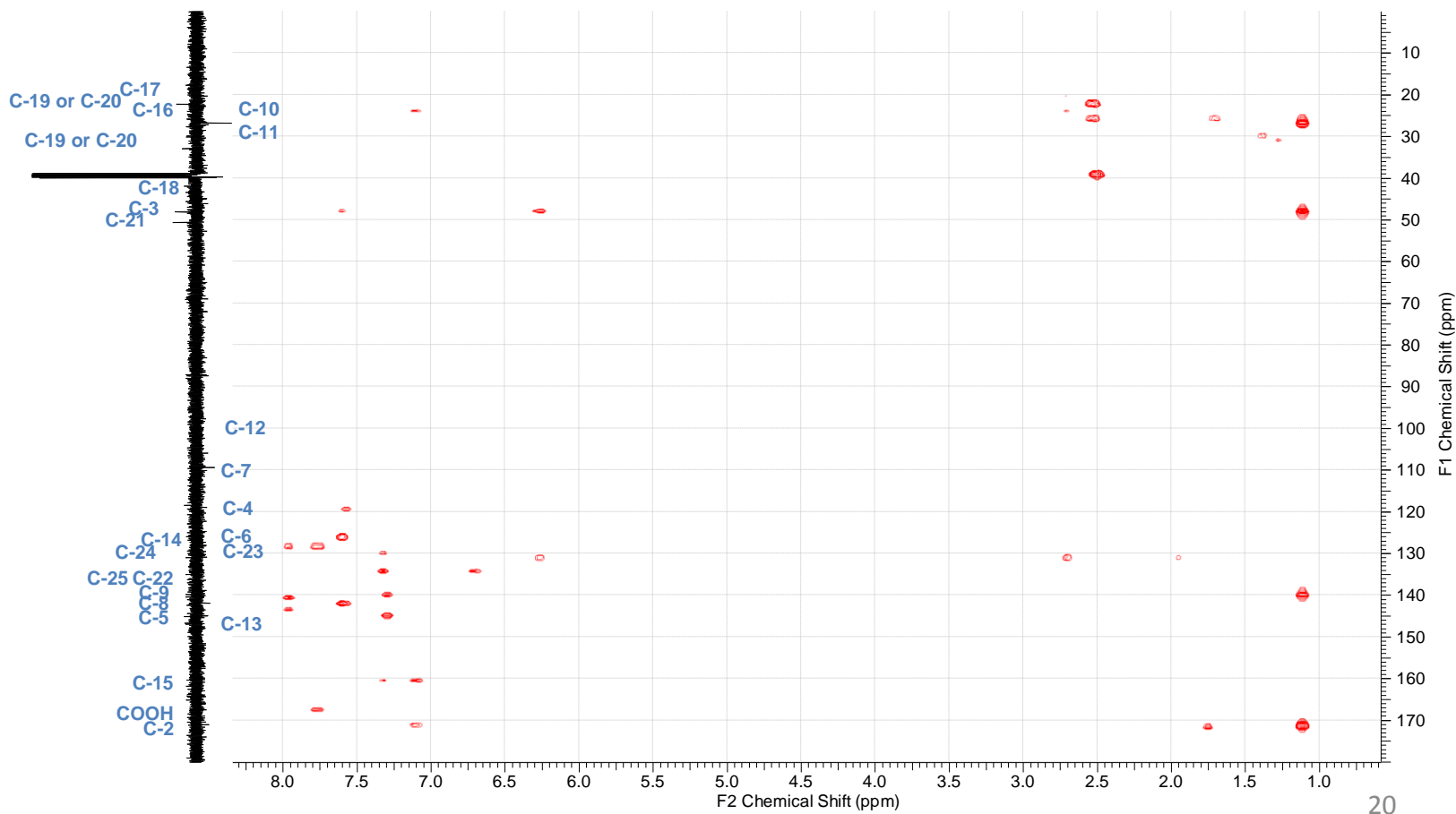
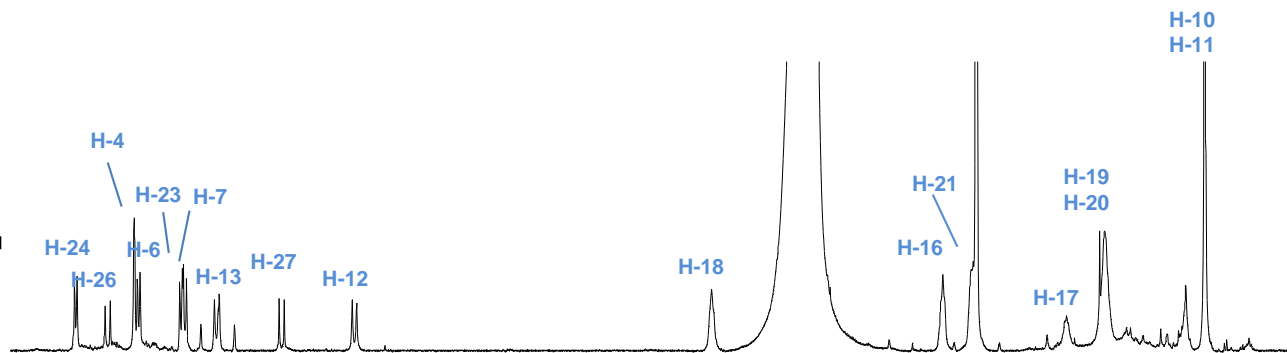
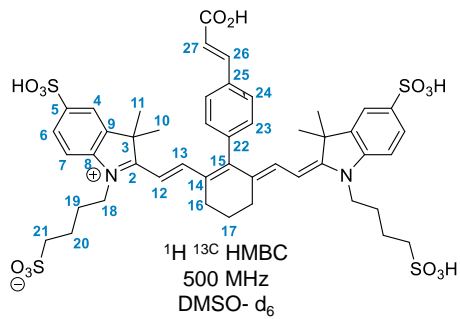


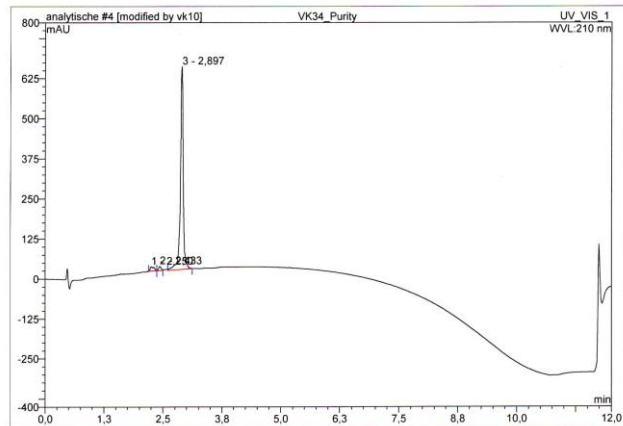
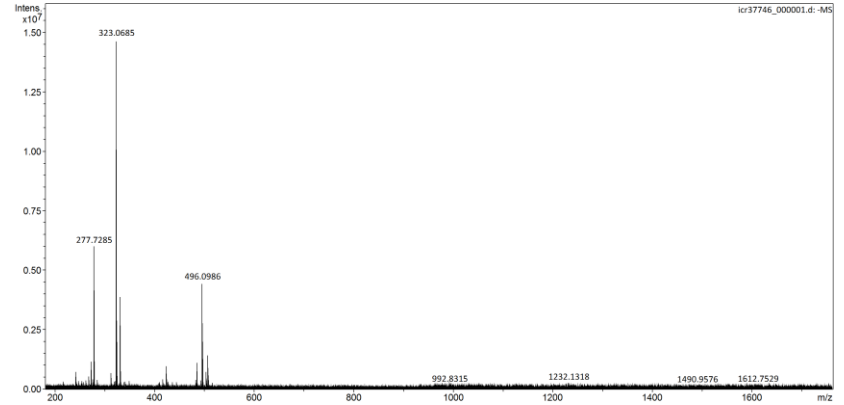
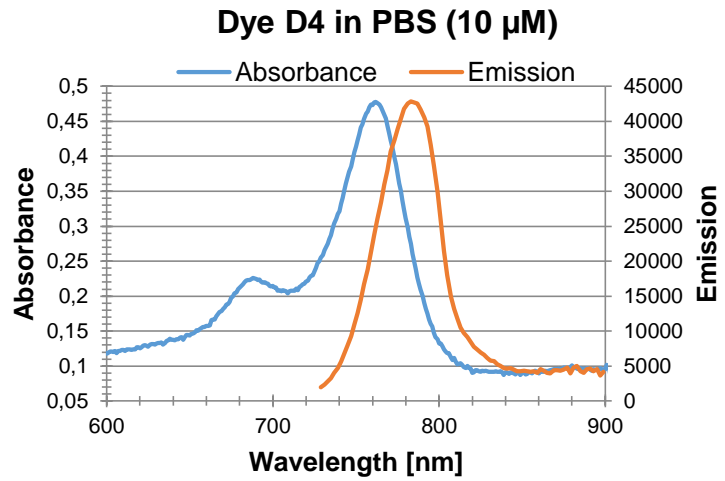
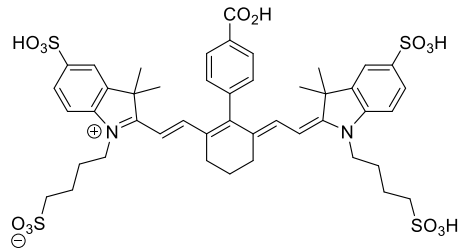




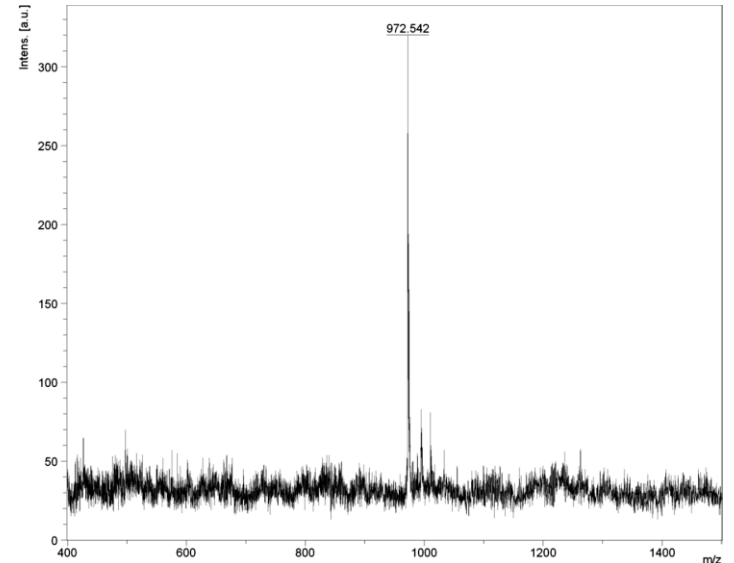


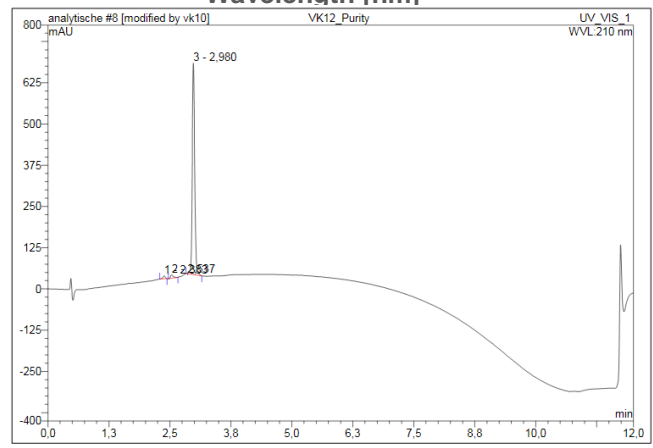
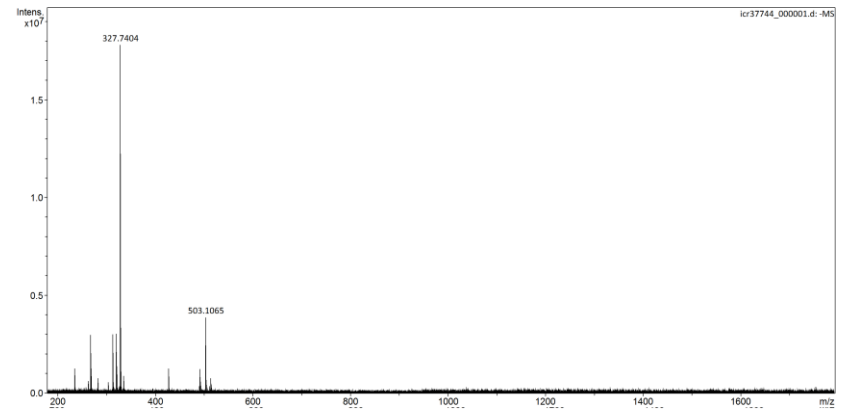
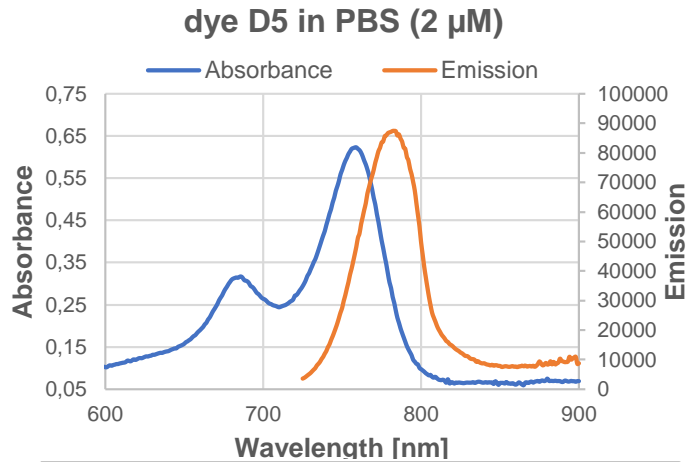
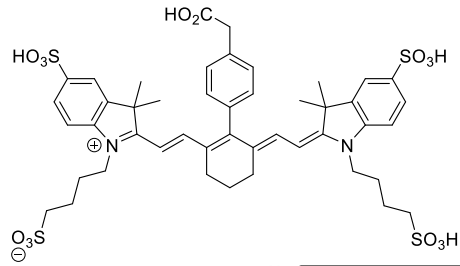




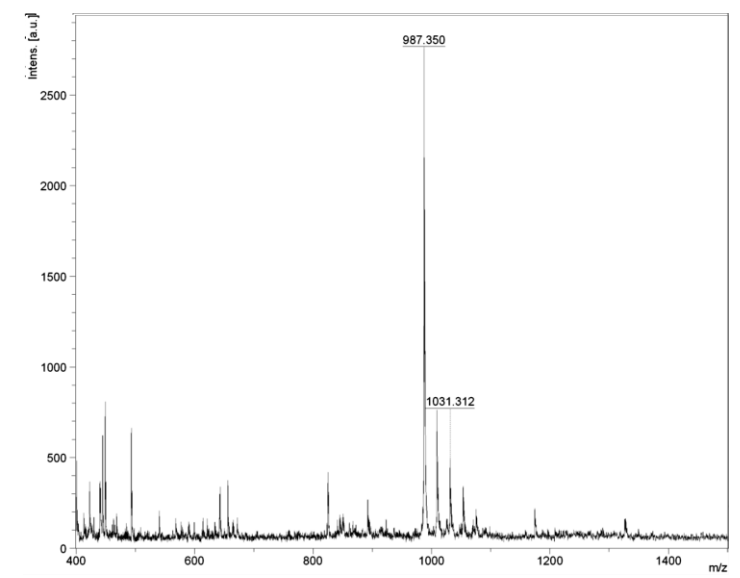


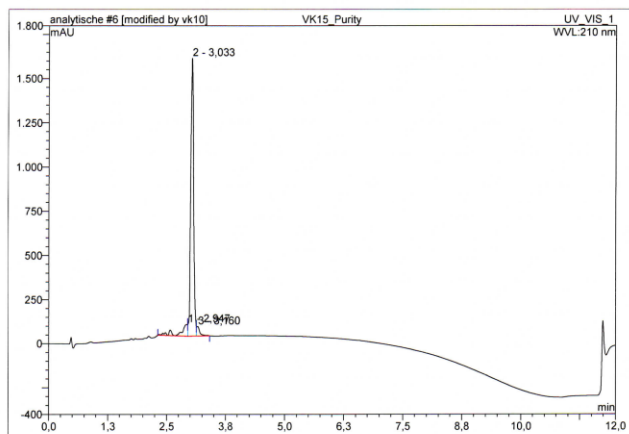
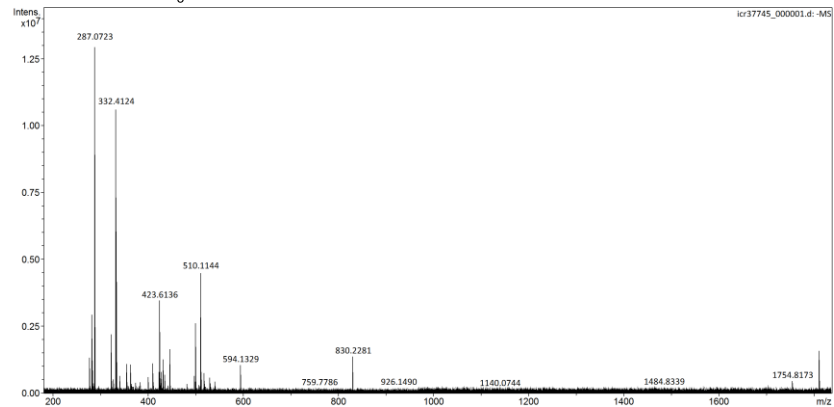
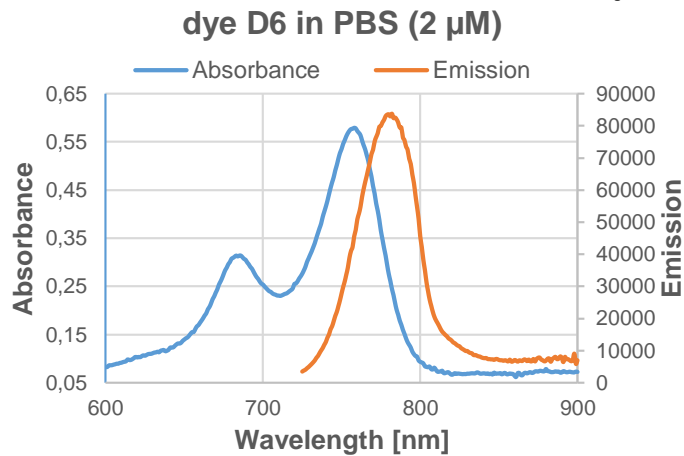
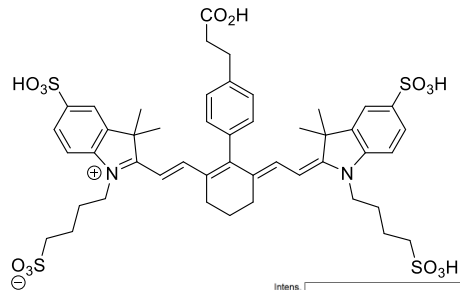
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2	2.43	n.a.	12,755	0,770	1,68	n.a.	M*
3	2.90	n.a.	631,986	43,942	95,71	n.a.	MB*
Total:			657,494	45,910	100,00	0,000	



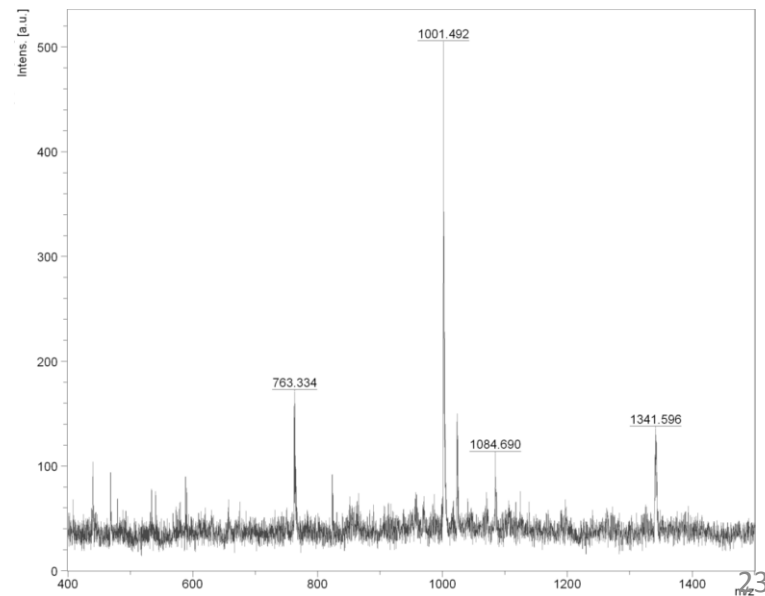


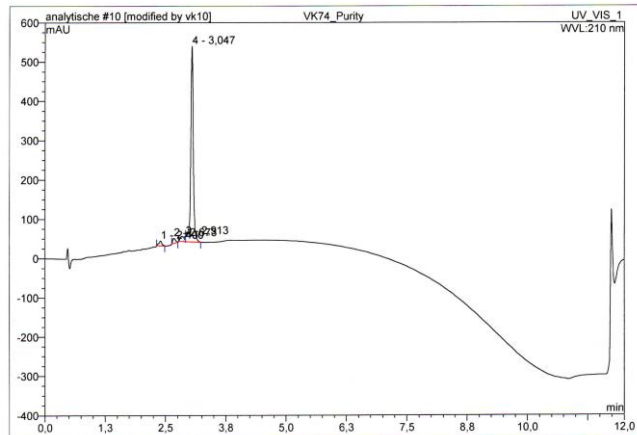
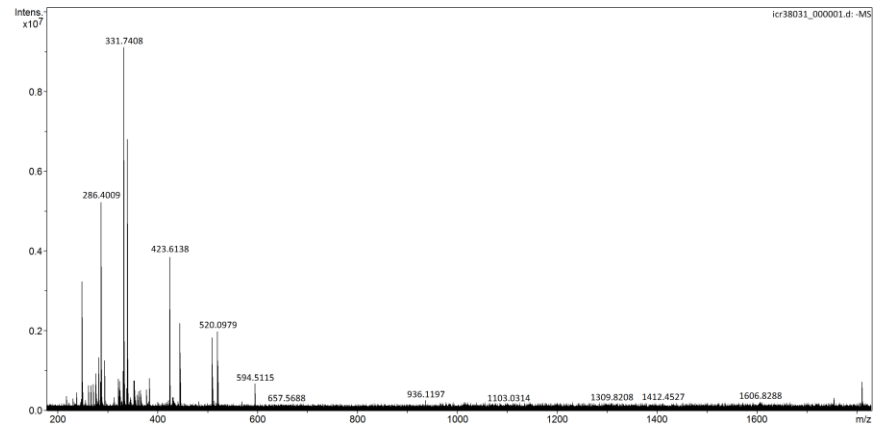
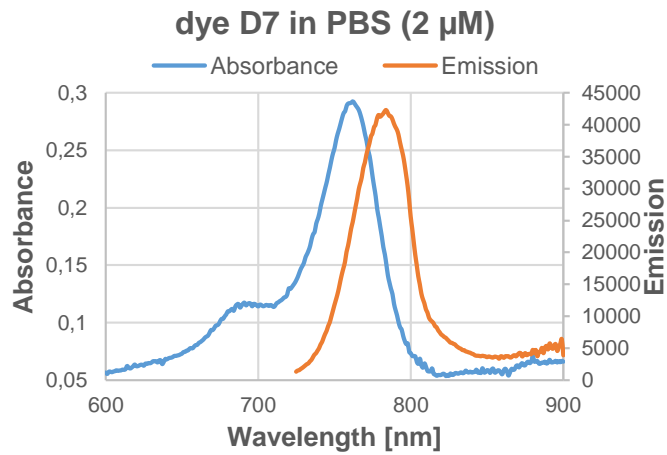
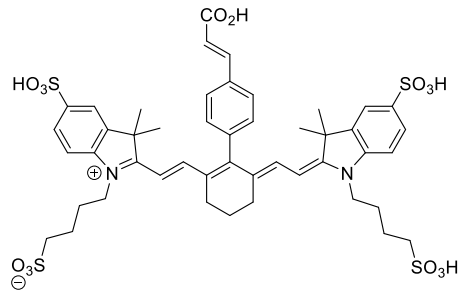
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2	2,54	n.a.	10,169	0,617	1,61	n.a.	BMB*
3	2,98	n.a.	641,207	37,126	97,06	n.a.	BMB*
Total:			660,045	38,252	100,00	0,000	



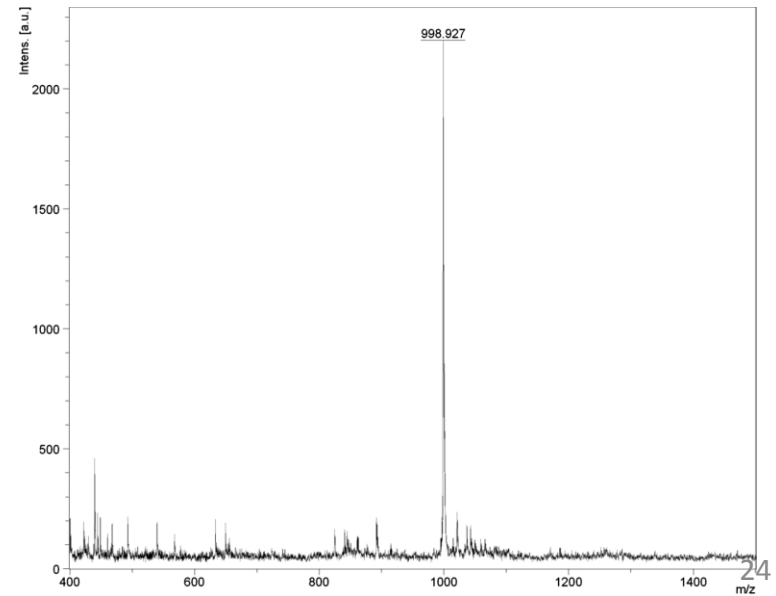


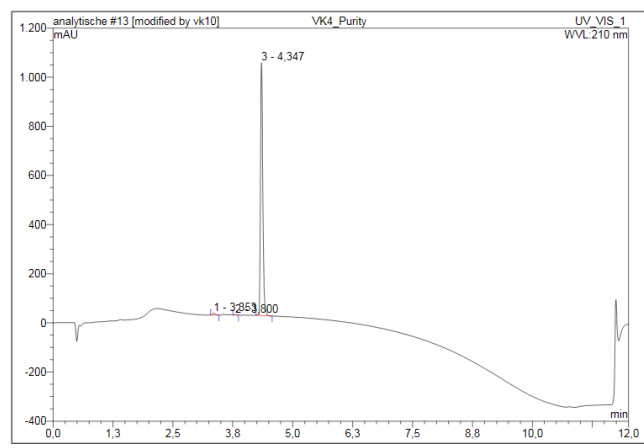
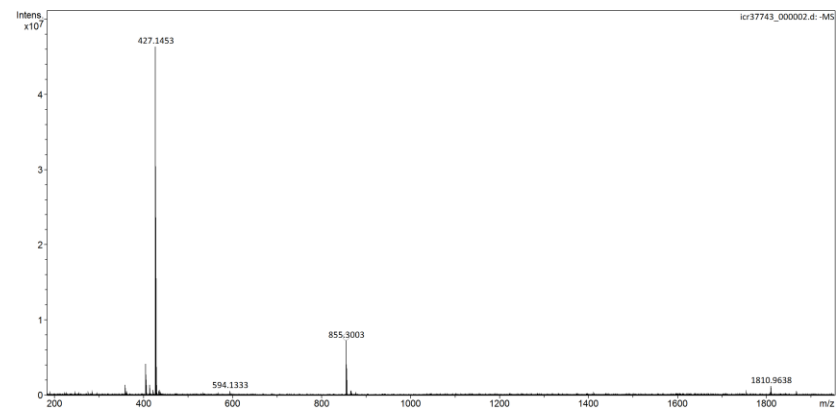
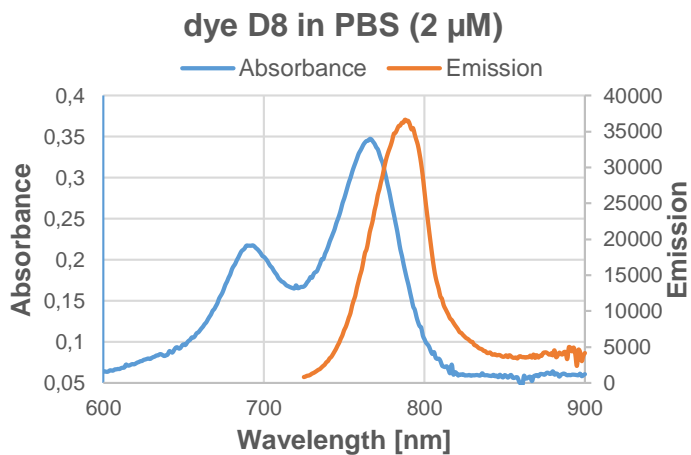
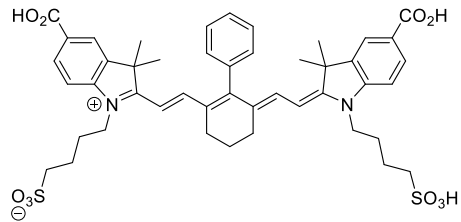
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	2,95	n.a	66,511	10,826	8,43	n.a	BM *
2	3,03	n.a	1571,761	113,399	88,30	n.a	M *
3	3,16	n.a	53,412	4,199	3,27	n.a	MB*
Total:			1691,684	128,424	100,00	0,000	



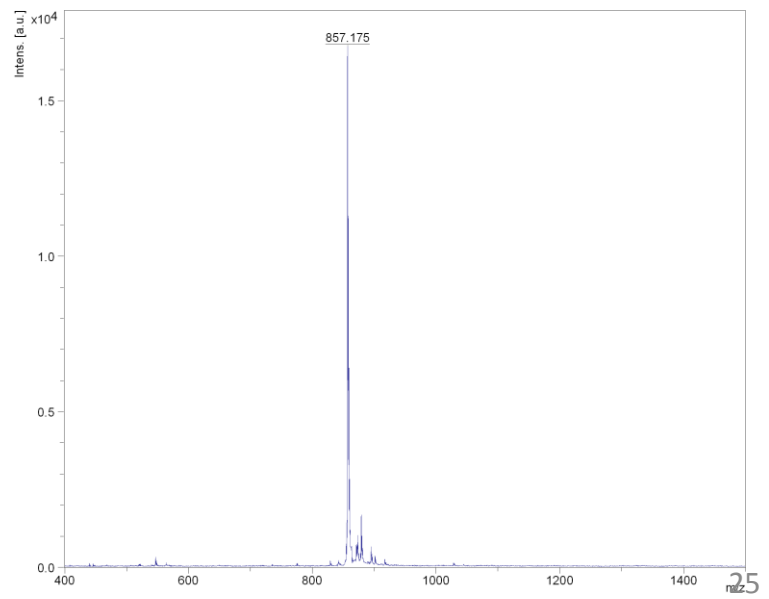


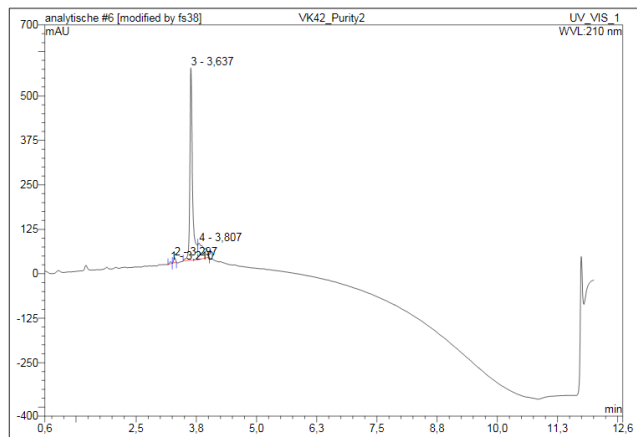
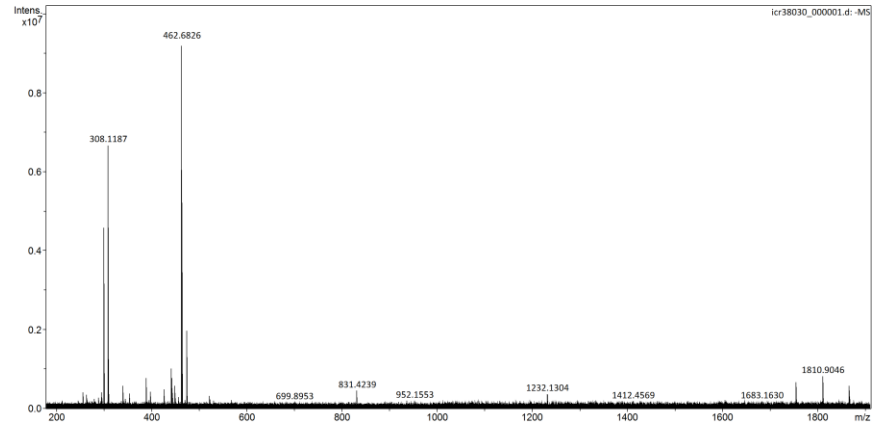
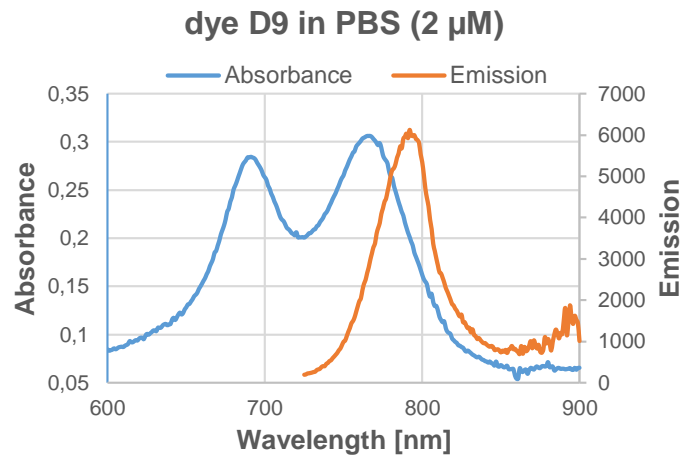
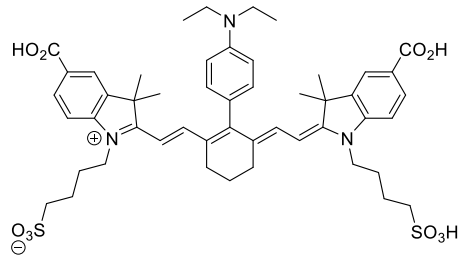
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	2.40	n.a.	11,766	0,834	2,49	n.a.	BMB*
2	2.67	n.a.	12,096	0,777	2,32	n.a.	BMB*
3	2.91	n.a.	13,349	1,380	4,12	n.a.	BM *
4	3.05	n.a.	497,864	30,523	91,08	n.a.	MB*
Total:			535,075	33,513	100,00	0,000	



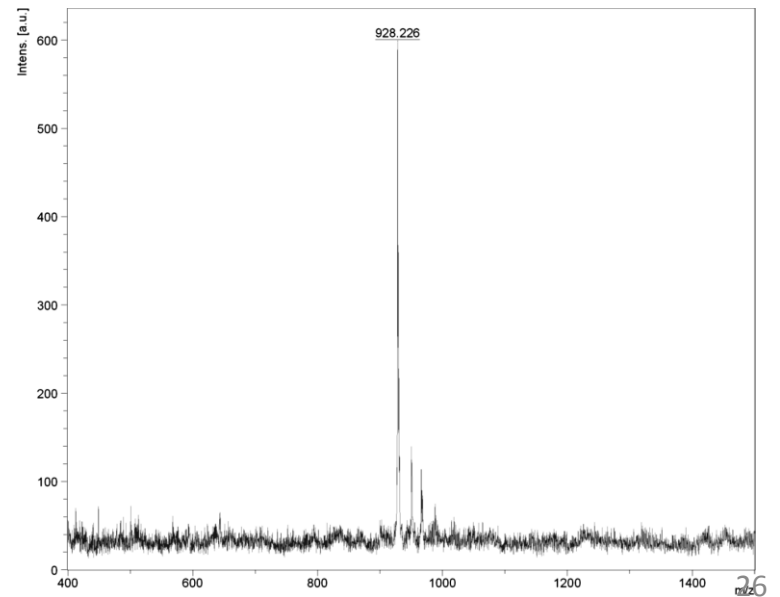


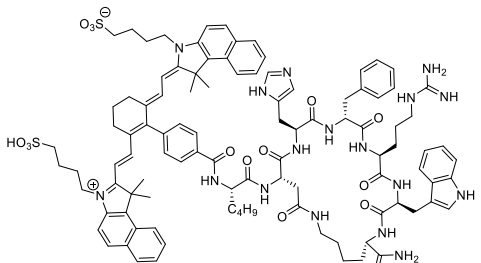
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3.35	n.a.	7.554	0.437	0.75	n.a.	BMB*
2	3.80	n.a.	1.530	0.069	0.12	n.a.	BMB*
3	4.35	n.a.	1028.743	57.367	99.13	n.a.	BMB*
Total:			1037.828	57.873	100.00	0.000	



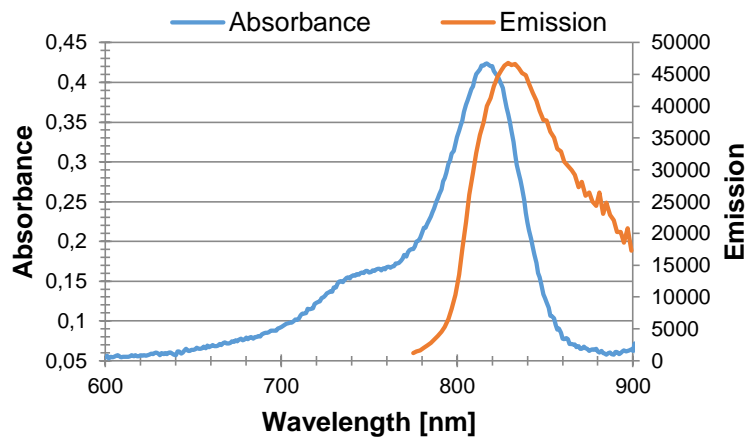


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3.21	n.a.	6,034	0,261	0,61	n.a.	BMB*
2	3,30	n.a.	13,941	0,586	1,37	n.a.	BMB*
3	3,64	n.a.	540,793	34,680	81,32	n.a.	BM *
4	3,81	n.a.	45,500	7,118	16,69	n.a.	MB*
Total:			606,267	42,646	100,00	0,000	

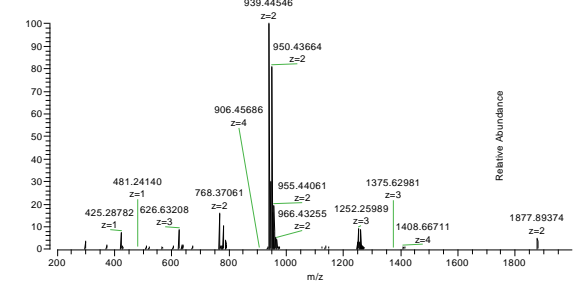




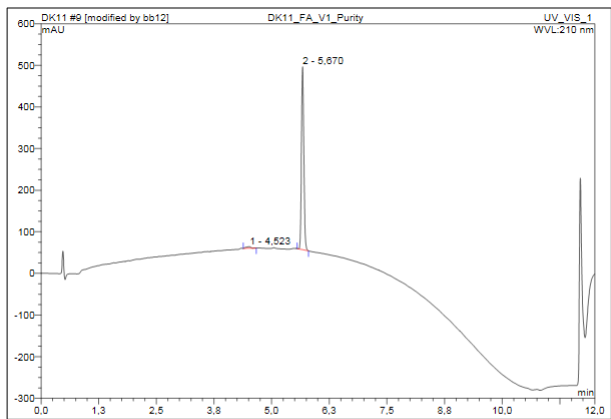
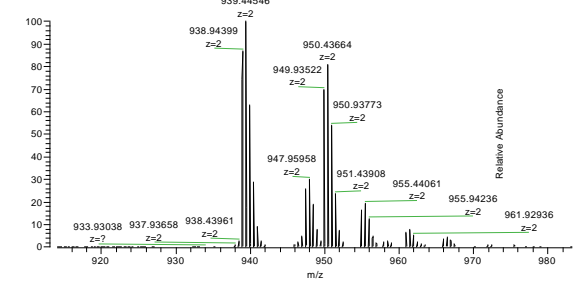
probe P1 in DMSO (1 μM)



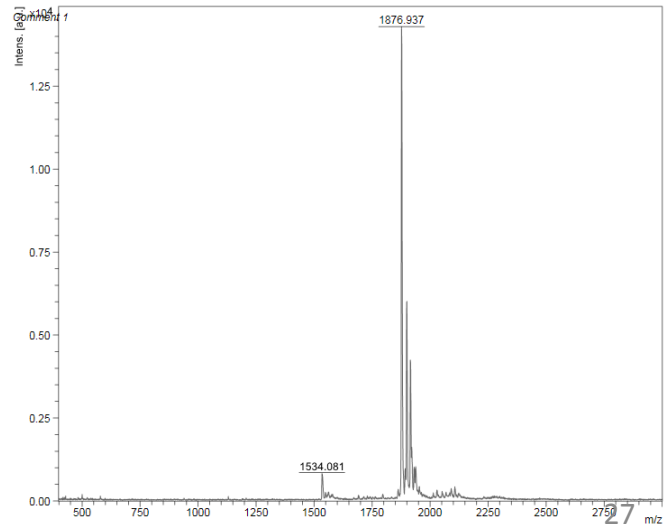
03-cwm-dk11 #54-270 RT: 0.53-2.43 AV: 27 NL: 2.86E5
 F: FTMS + p ESI Full ms [200.00-2000.00]

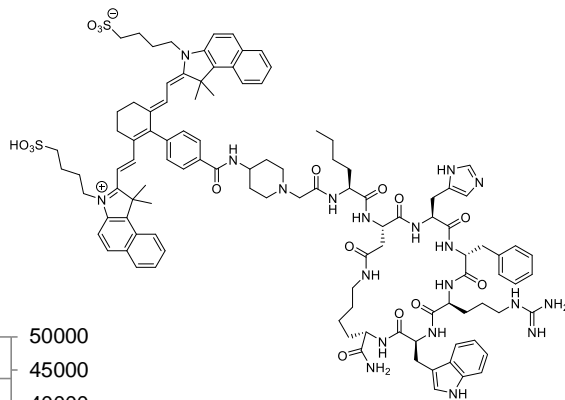


03-cwm-dk11 #54-270 RT: 0.53-2.43 AV: 27 NL: 2.86E5
 F: FTMS + p ESI Full ms [200.00-2000.00]

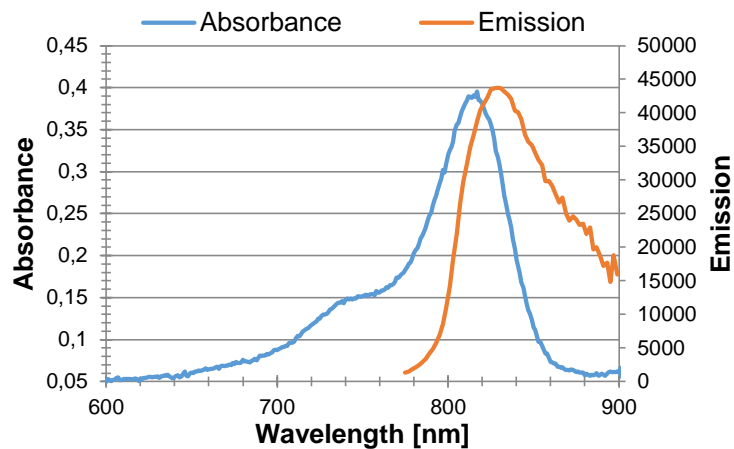


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	4.52	n.a.	3,608	0,458	1,70	n.a.	BMB ⁺
2	5,67	n.a.	439,602	26,549	98,30	n.a.	BMB ⁺
Total:			443,210	27,008	100,00	0,000	

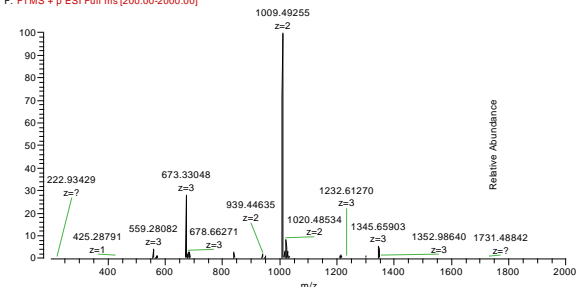




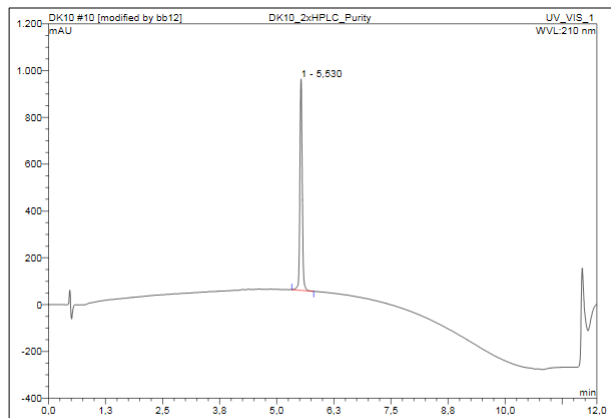
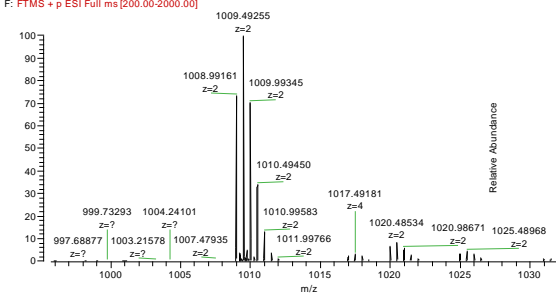
probe P2 in DMSO (1 μ M)



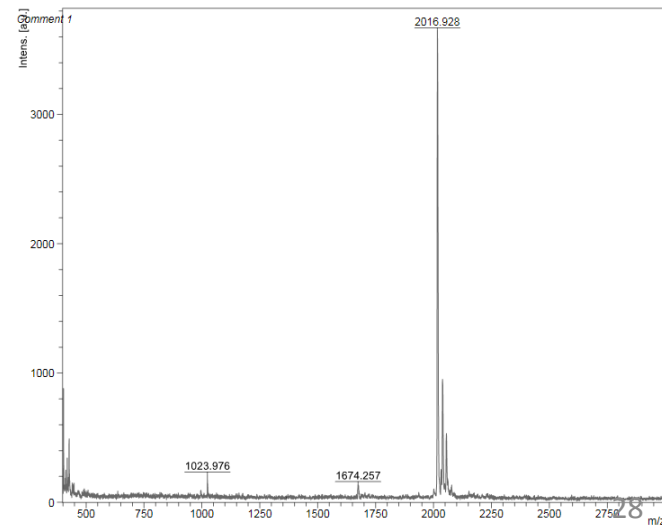
03-cwm-dk10 #53-279 RT: 0.55-2.43 AV: 28 NL: 3.00E6
F: FTMS + p ESI Full ms [200.00-2000.00]

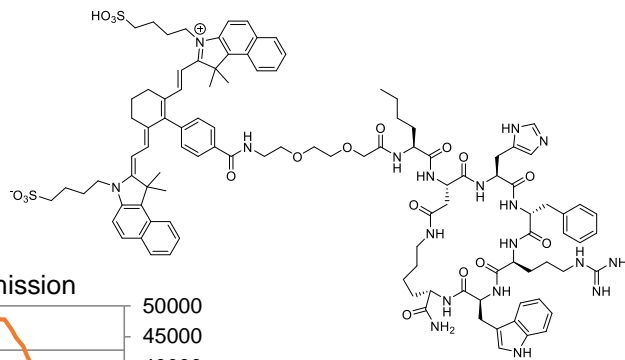


03-cwm-dk10 #53-279 RT: 0.55-2.43 AV: 28 NL: 3.00E6
F: FTMS + p ESI Full ms [200.00-2000.00]

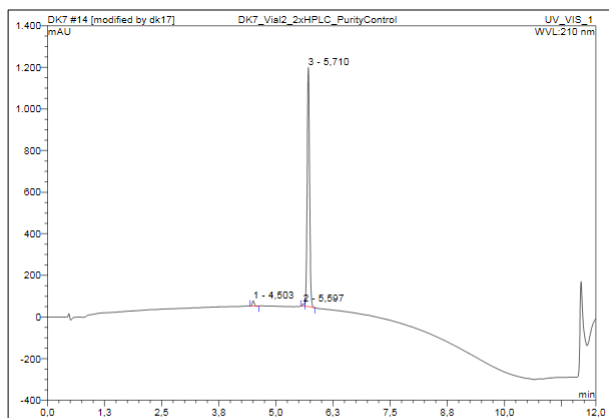
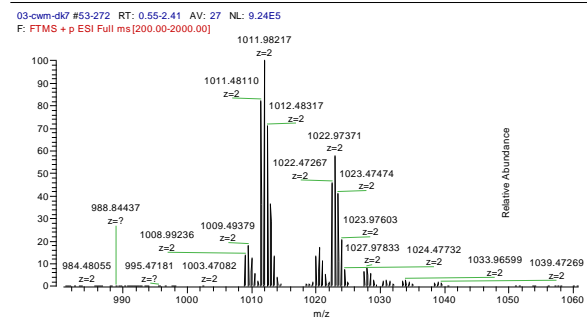
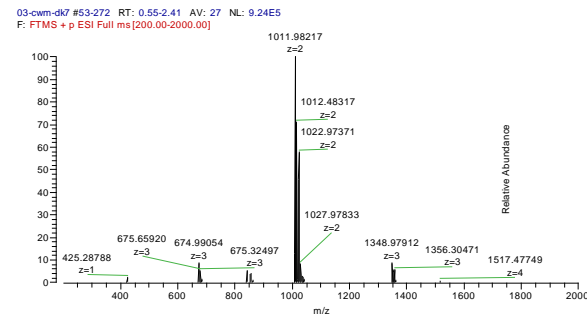
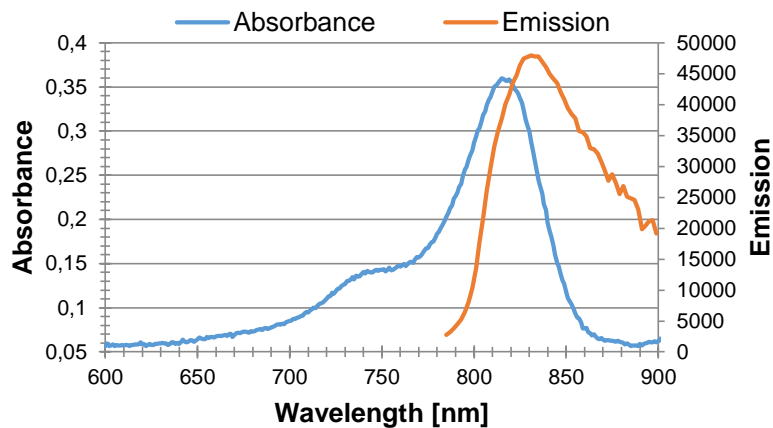


No.	Ret. Time min	Peak Name	Height mAU	Area mAU*min	Rel. Area %	Amount	Type
1	5.53	n.a.	902.925	54.295	100.00	n.a.	BMB*
Total:			902.925	54.295	100.00	0.000	

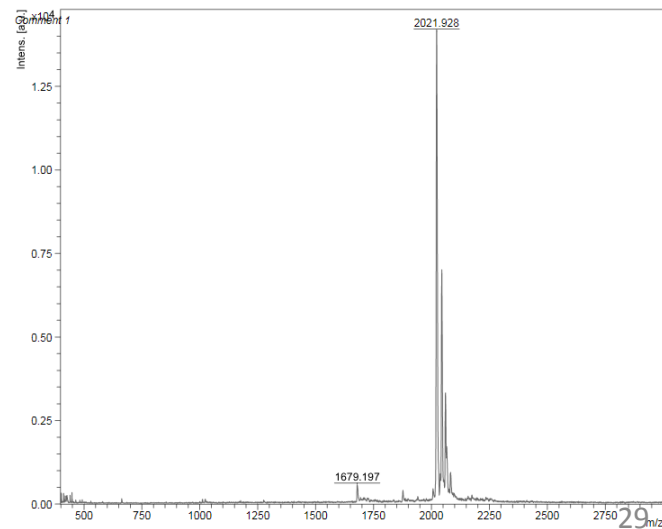


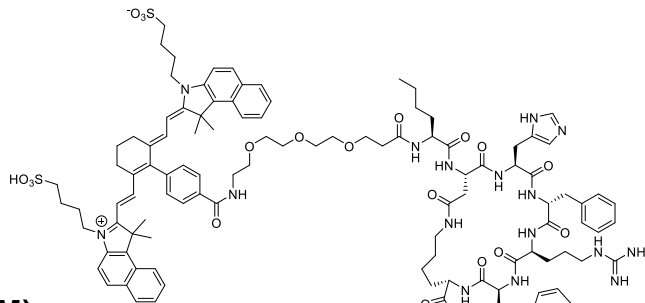


probe P3 in DMSO (1 μ M)

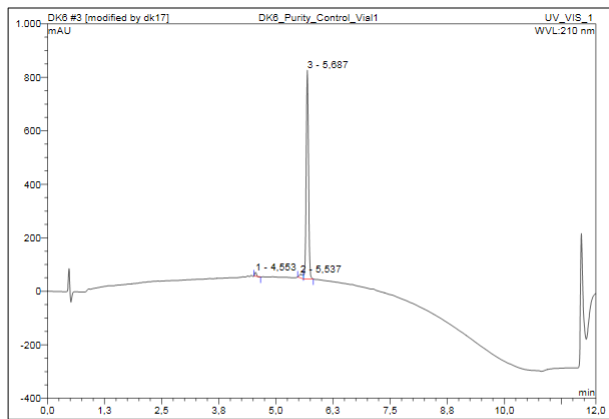
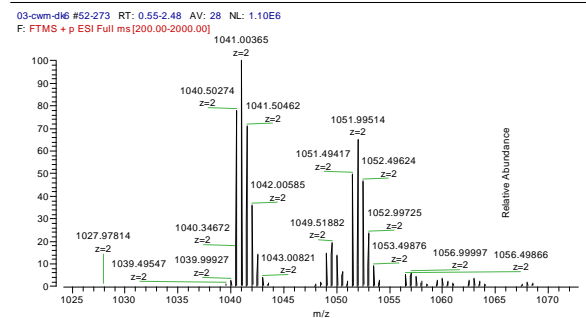
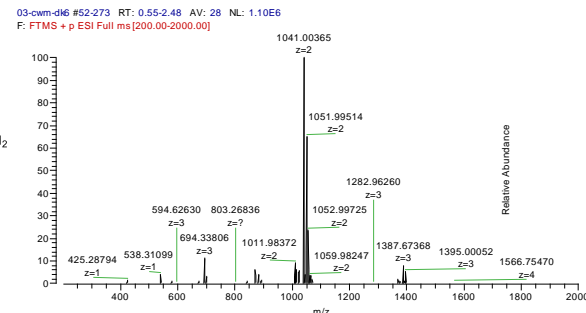
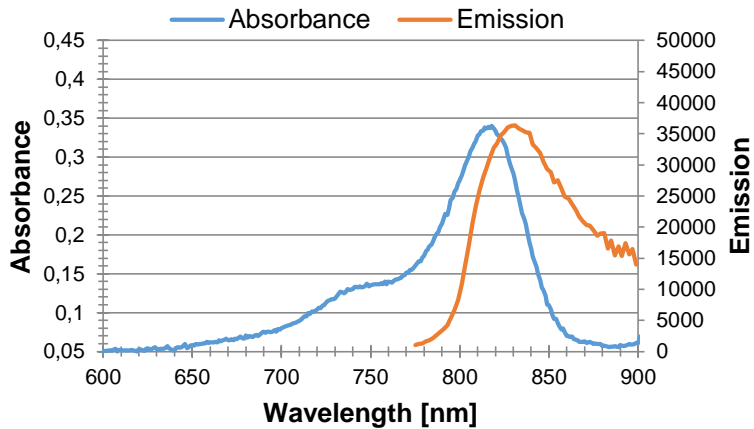


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	4,50	n.a.	24,748	1,223	1,69	n.a.	BMB*
2	5,60	n.a.	9,145	0,562	0,78	n.a.	BM *
3	5,71	n.a.	1149,851	70,534	97,53	n.a.	MB*
Total:			1183,745	72,319	100,00	0,000	

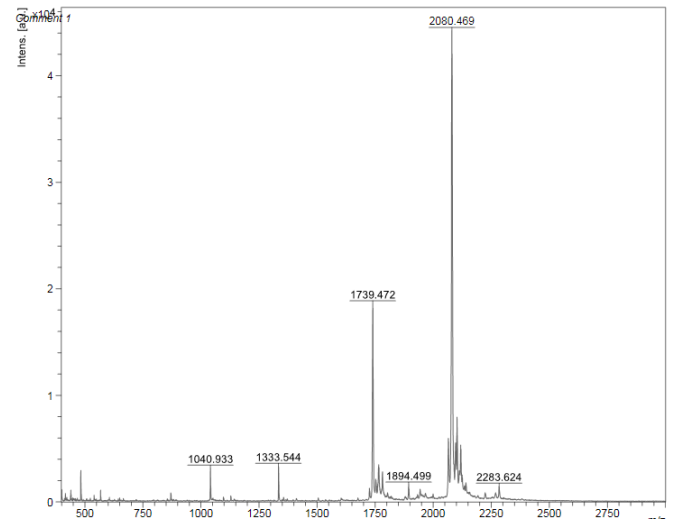


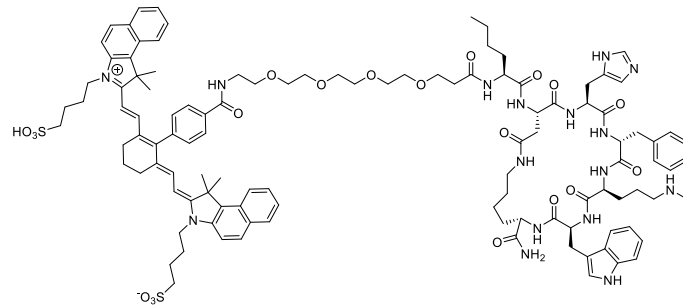


probe P4 in DMSO (1 μM)

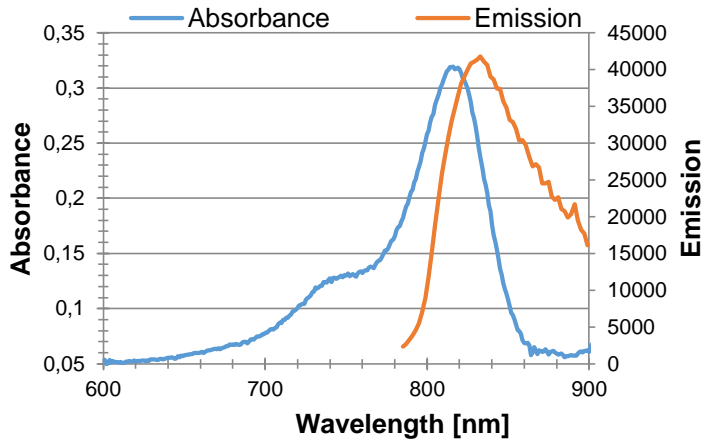


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	4,55	n.a.	14,330	0,564	1,17	n.a.	BMB*
2	5,54	n.a.	12,970	1,347	2,79	n.a.	BM *
3	5,69	n.a.	780,042	46,361	96,04	n.a.	MB*
Total:			807,343	48,273	100,00	0,000	

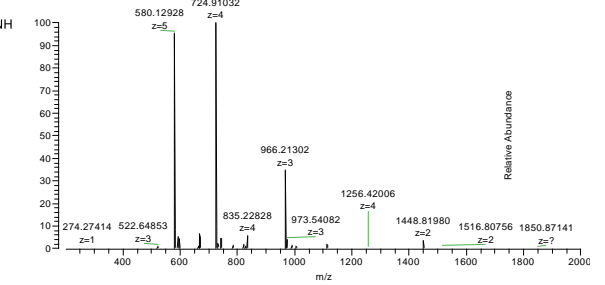




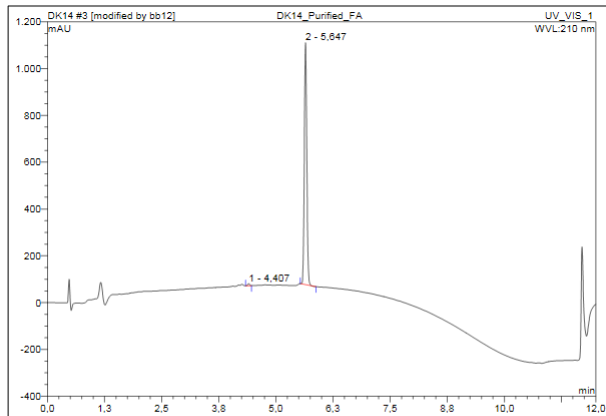
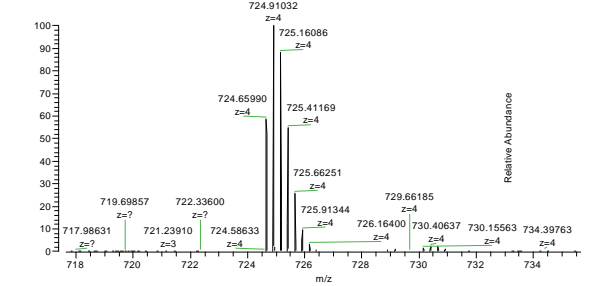
probe P5 in DMSO (1 μ M)



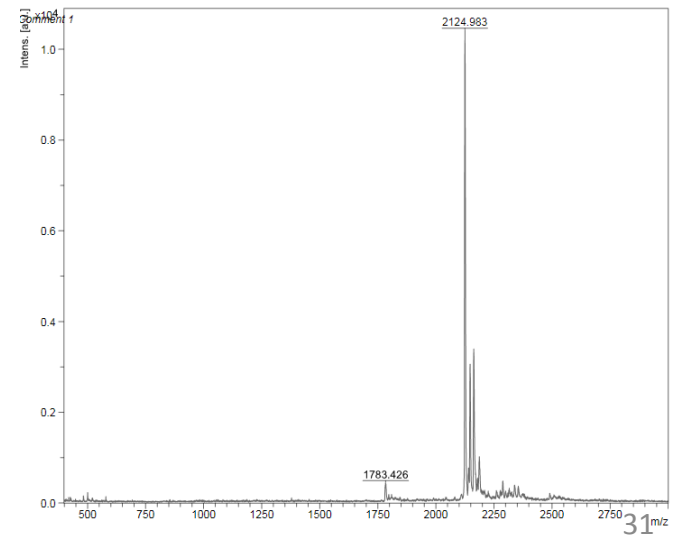
03-cwm-DK14 #52-285 RT: 0.55-2.45 AV: 29 NL: 1.63E7
F: FTMS + p ESI Full ms [200.00-2000.00]

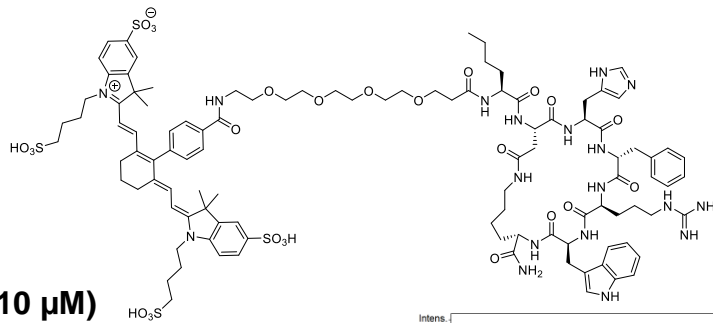


03-cwm-DK14 #52-285 RT: 0.55-2.45 AV: 29 NL: 1.63E7
F: FTMS + p ESI Full ms [200.00-2000.00]

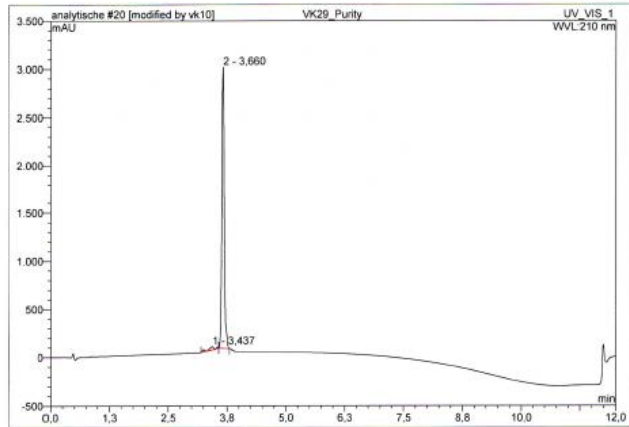
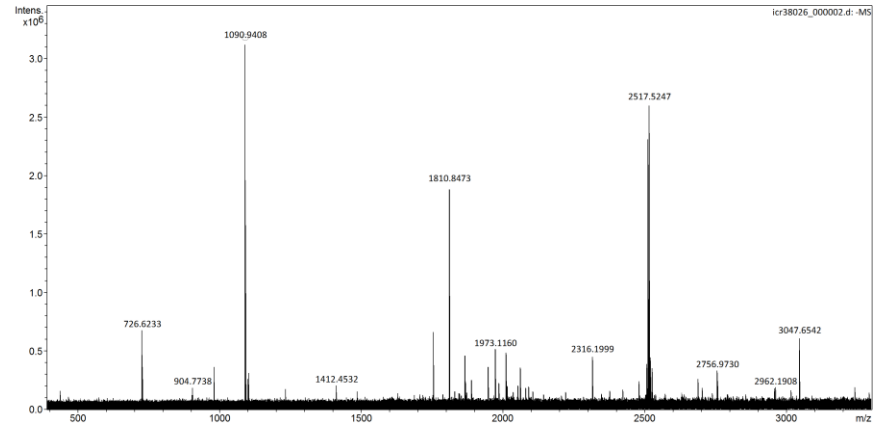
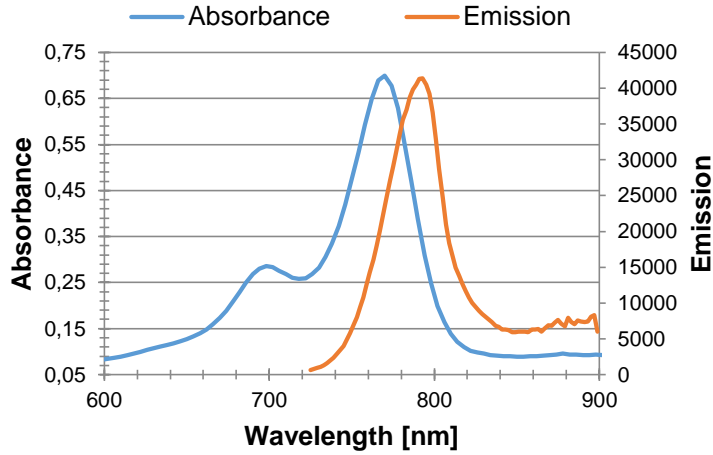


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	4,41	n.a.	8,728	0,446	0,67	n.a.	BMB*
2	5,65	n.a.	1033,343	65,592	99,33	n.a.	BMB*
Total:			1042,071	66,037	100,00	0,000	

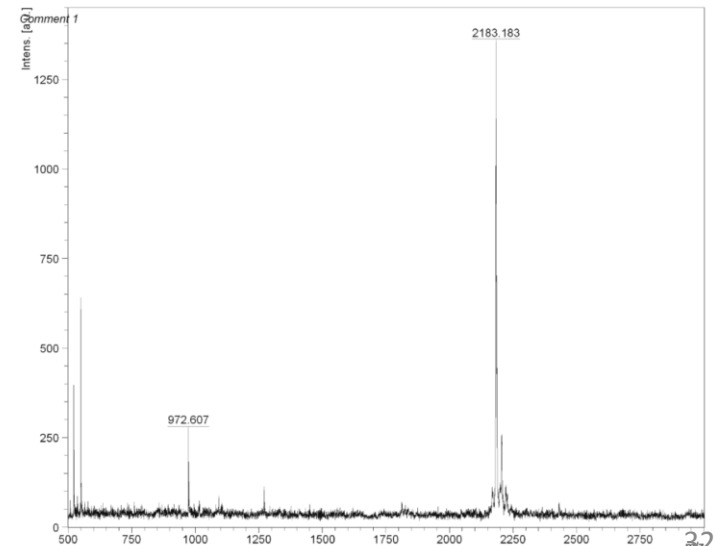


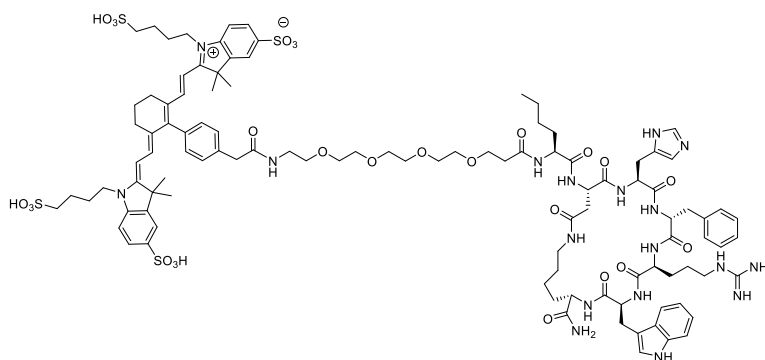


probe P6 in PBS (10 μ M)

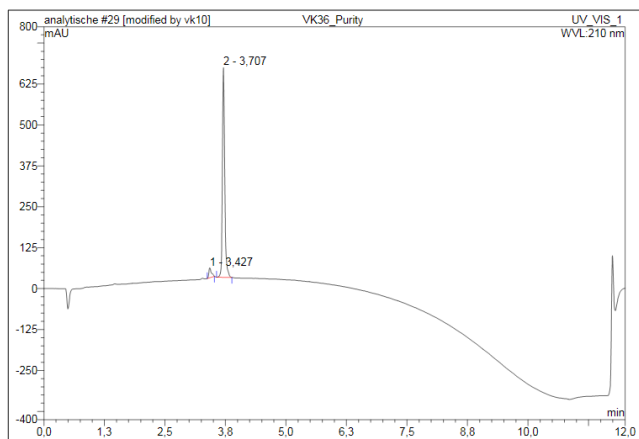
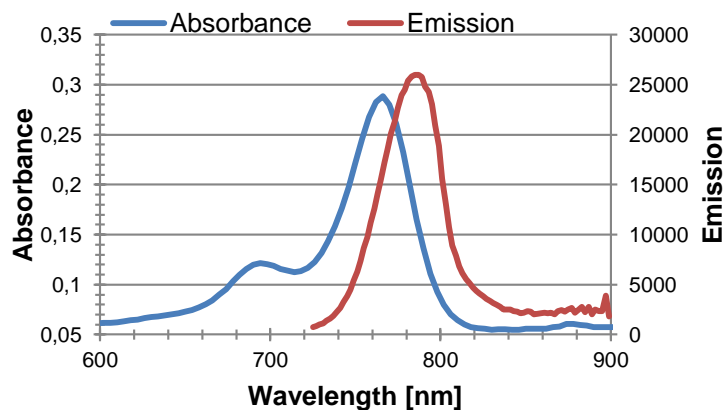


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3.44	n.a.	31.409	4.360	2.57	n.a.	BMB*
2	3.66	n.a.	2926.110	165.499	97.43	n.a.	bMB*
Total:			2957.519	169.859	100.00	0.000	

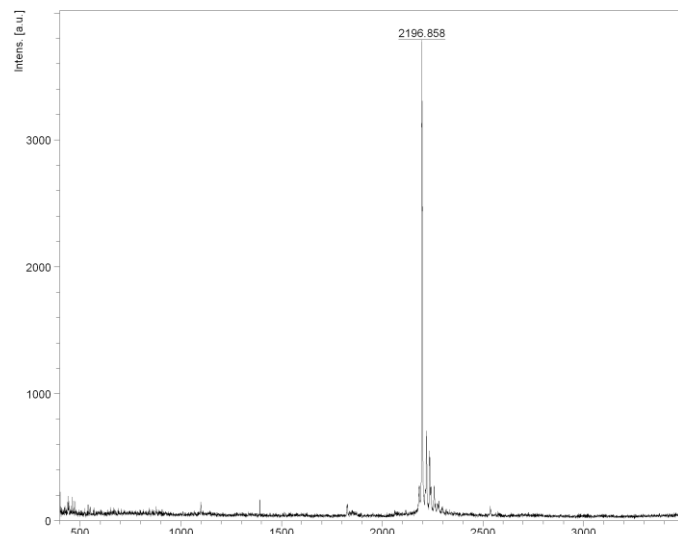


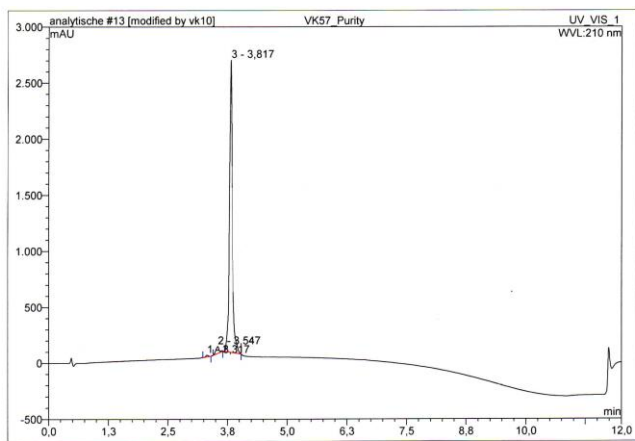
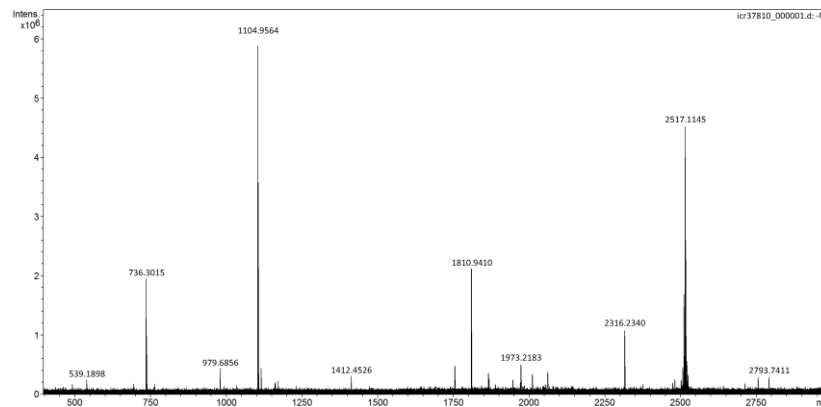
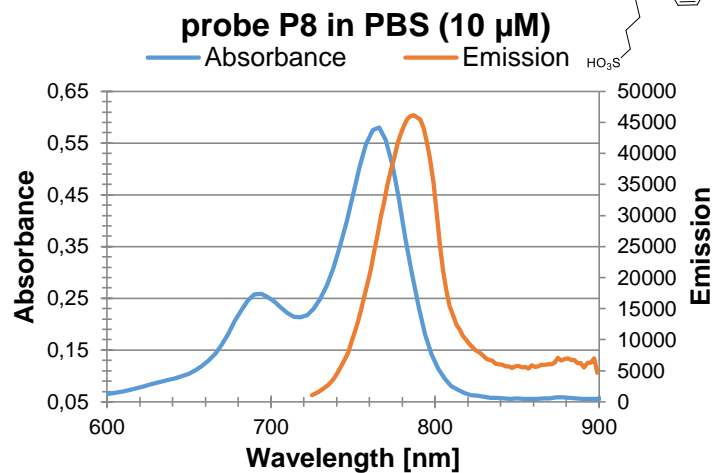
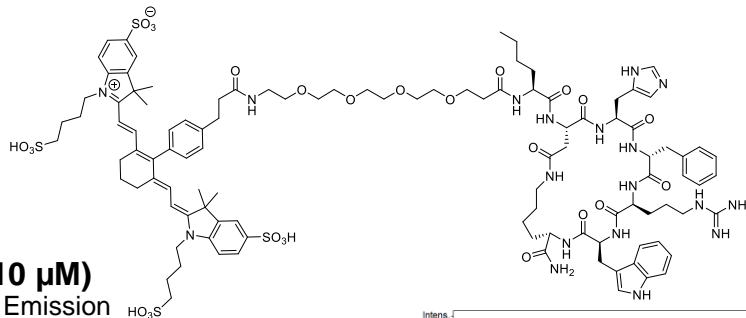


probe P7 in PBS (10 μ M)

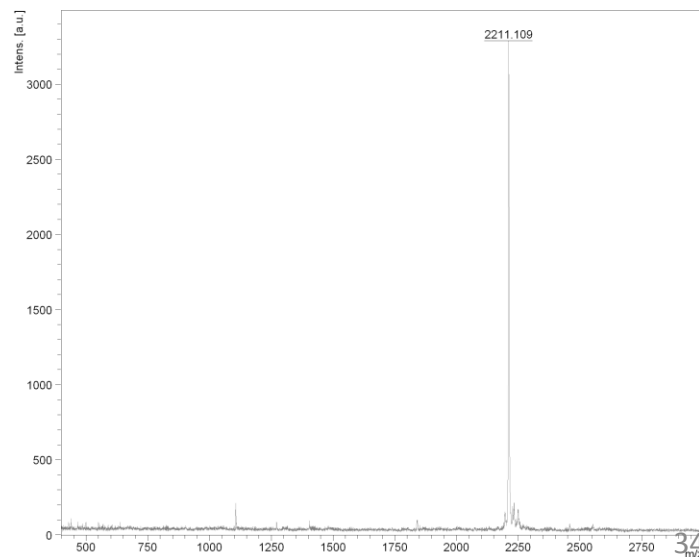


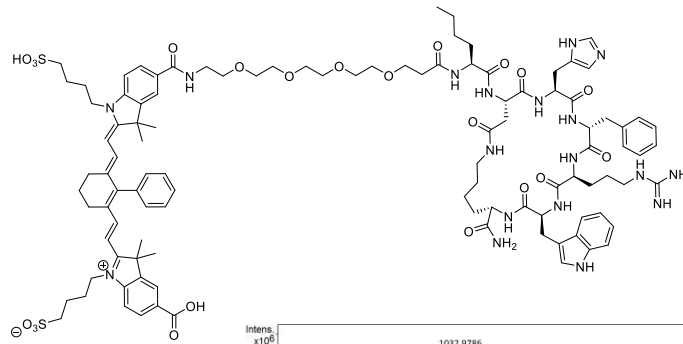
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3.43	n.a.	29,868	1,855	4,91	n.a.	BMB*
2	3.71	n.a.	640,543	35,955	95,09	n.a.	BMB*
Total:			670,411	37,810	100,00	0,000	



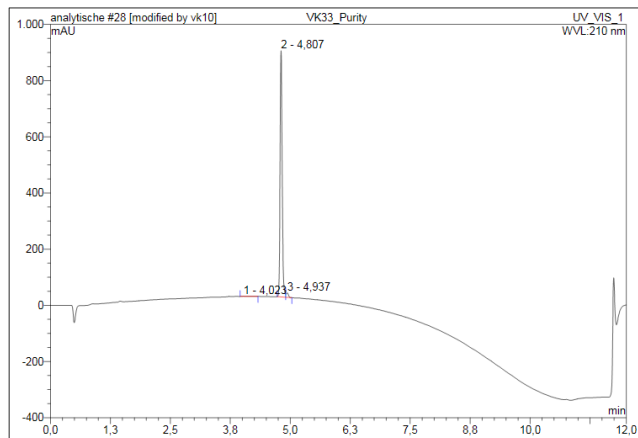
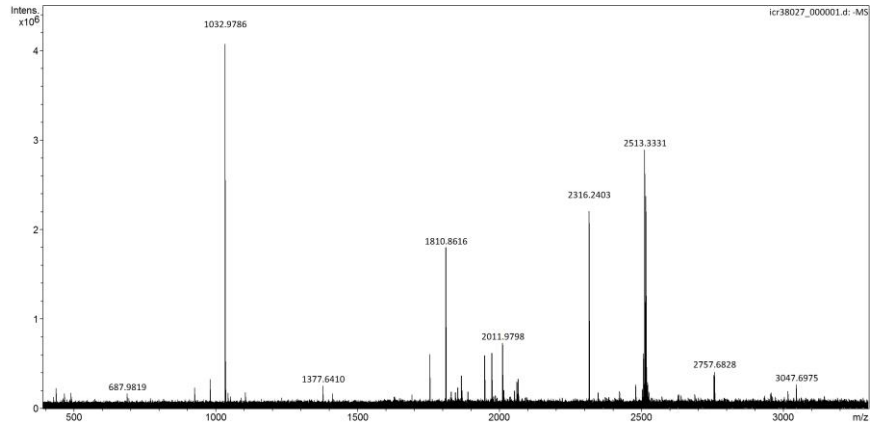
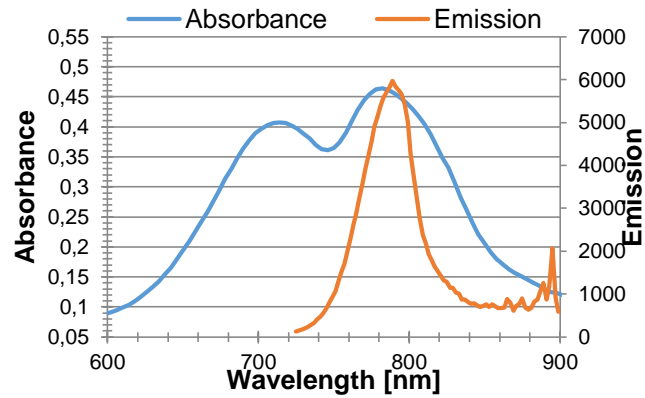


No.	Ret. Time min	Peak Name	Height mAU	Area mAU*min	Rel. Area %	Amount	Type
1	3,32	n.a.	14,907	0,710	0,37	n.a.	BMB*
2	3,55	n.a.	62,586	5,042	2,62	n.a.	BMB*
3	3,82	n.a.	2608,939	186,514	97,01	n.a.	BMB*
Total:			2686,431	192,266	100,00	0,000	

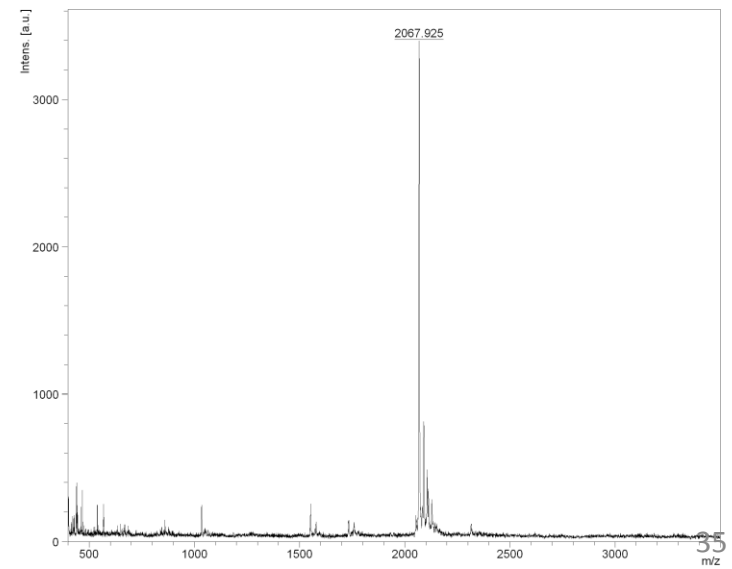


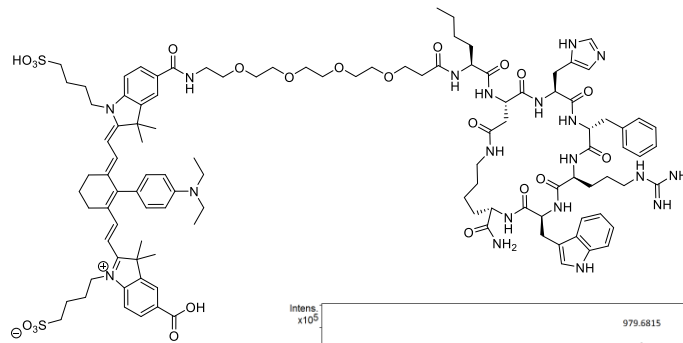


probe P9 in PBS (20 μM)

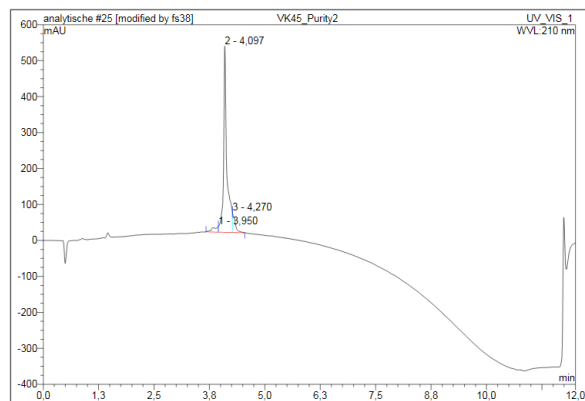
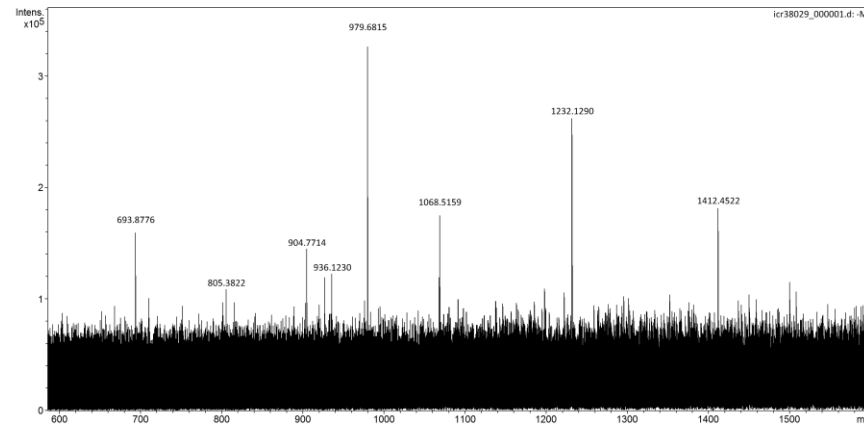
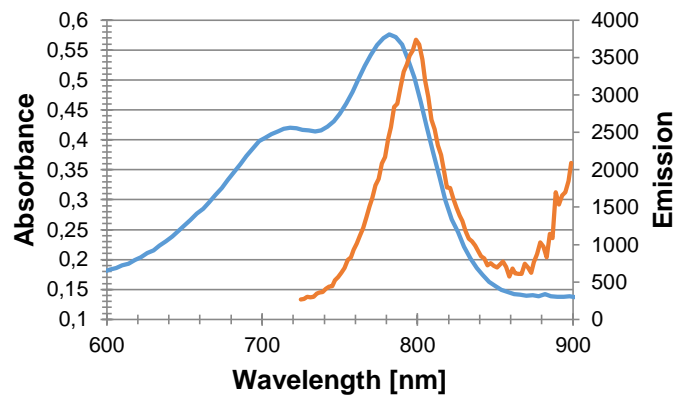


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	4,02	n.a.	1,088	0,135	0,30	n.a.	BMB*
2	4,81	n.a.	876,267	44,783	97,74	n.a.	BM *
3	4,94	n.a.	15,632	0,898	1,96	n.a.	MB*
Total:			892,986	45,817	100,00	0,000	

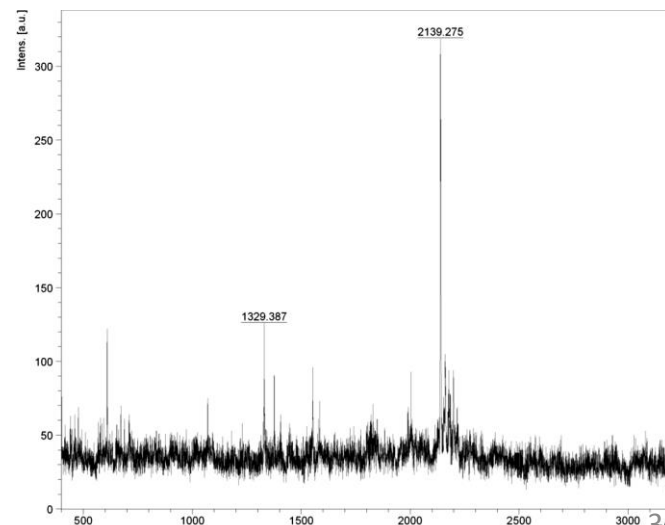


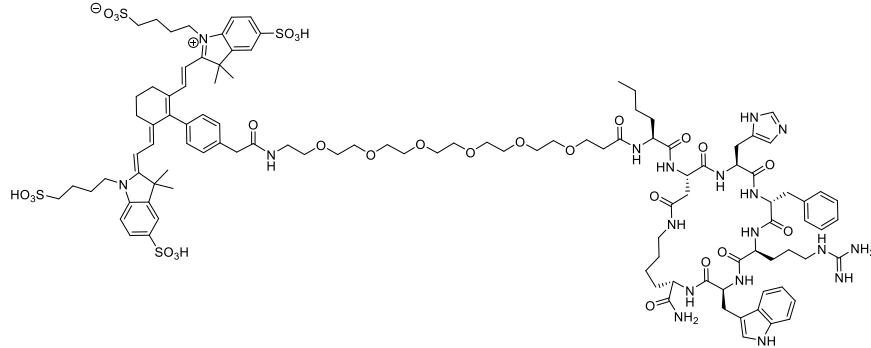


probe P10 in PBS (20 μ M)
 — Absorbance — Emission

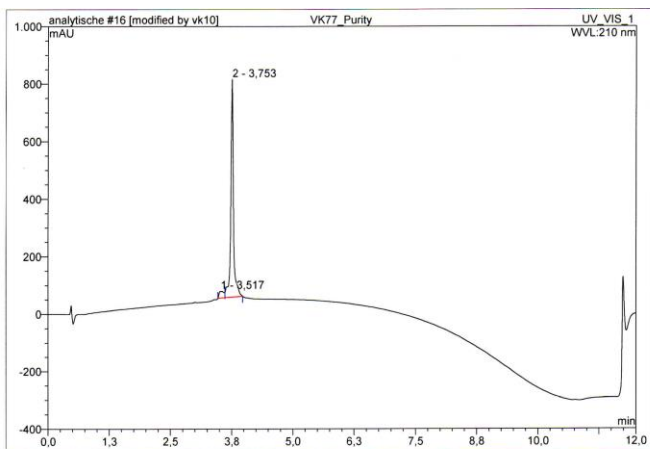
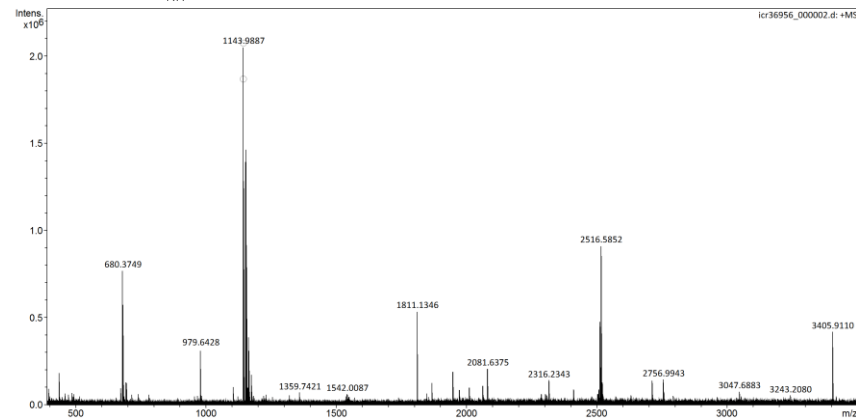
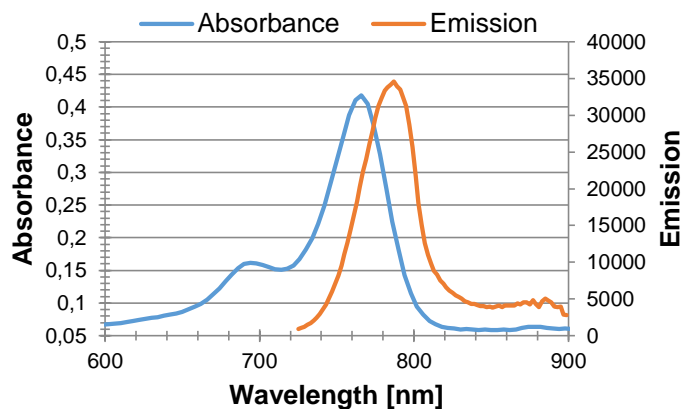


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3.95	n.a.	16.125	2,106	4,18	n.a.	BM *
2	4.10	n.a.	517,984	44,517	88,44	n.a.	M *
3	4.27	n.a.	54,583	3,713	7,38	n.a.	MB*
Total:			588,692	50,336	100,00	0,000	

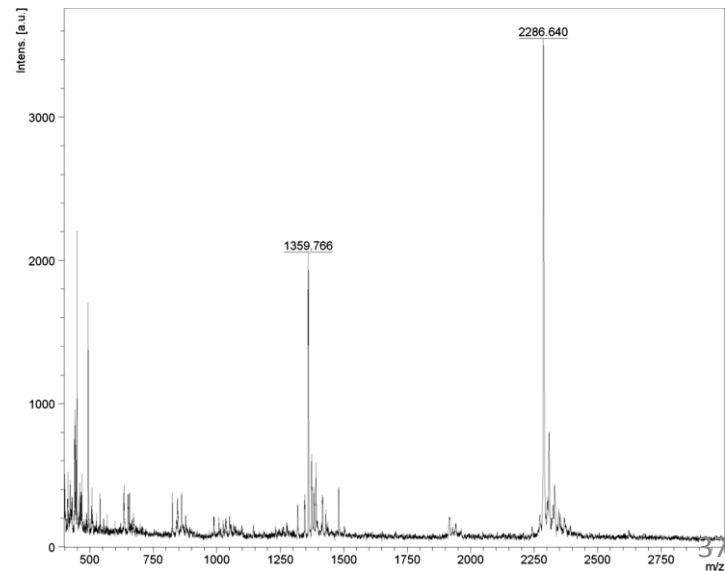


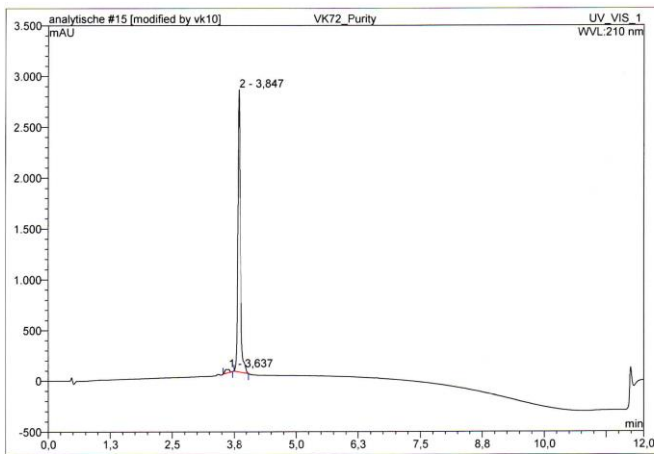
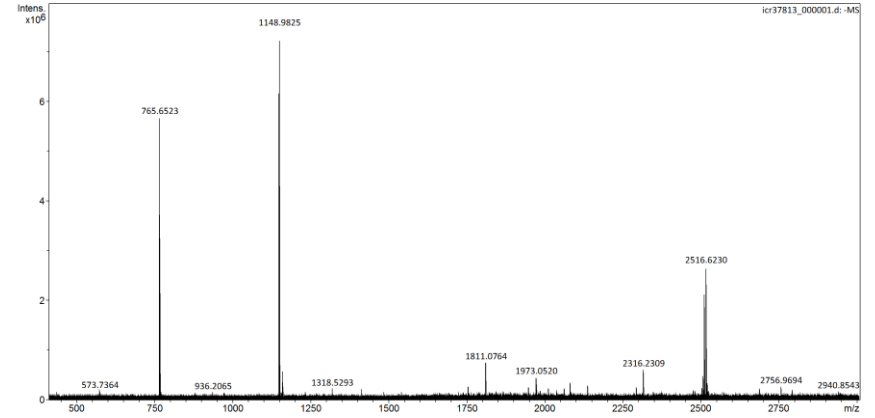
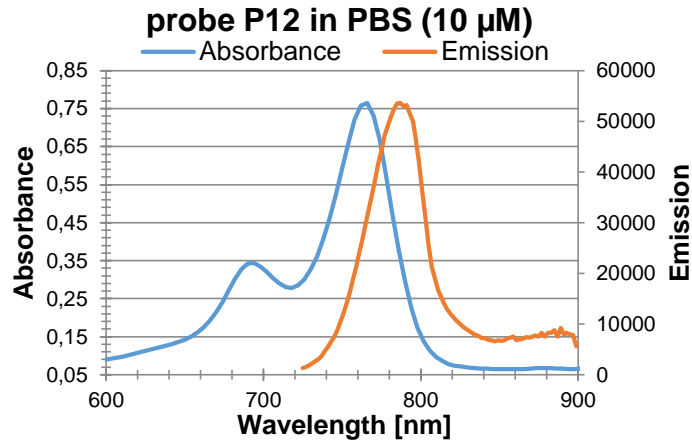
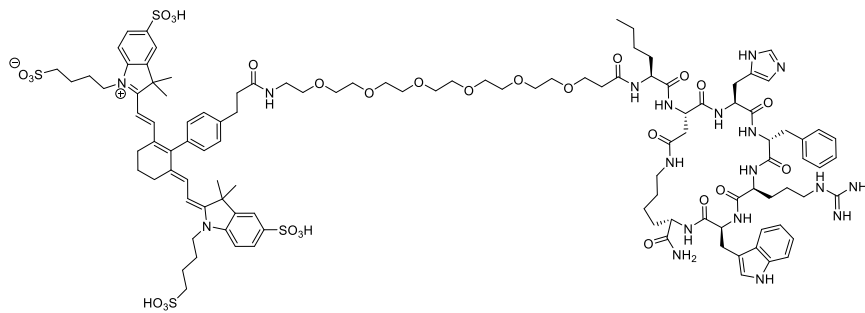


probe 11 in PBS (10 μ M)

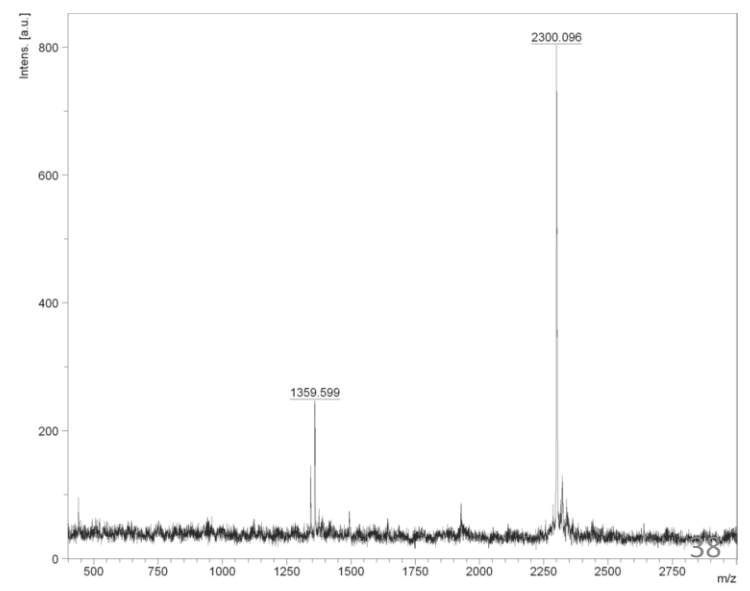


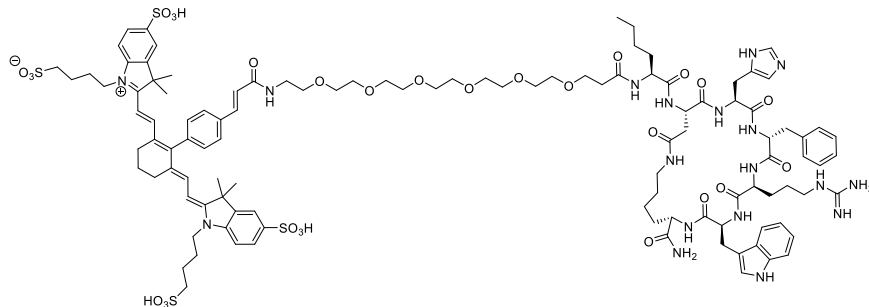
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3,52	n.a.	23,550	2,547	4,94	n.a.	BM *
2	3,75	n.a.	756,113	49,052	95,06	n.a.	MB*
Total:			779,664	51,598	100,00	0,000	



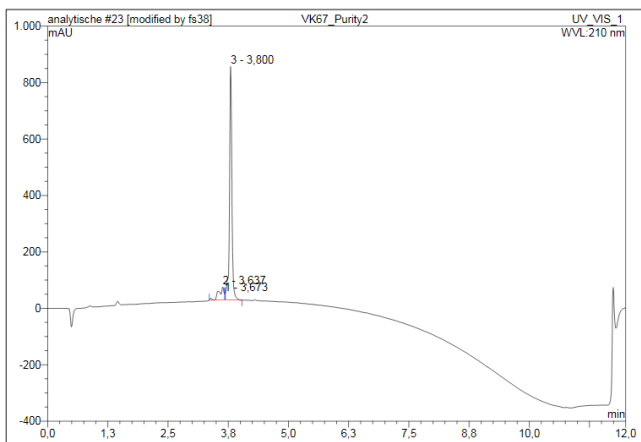
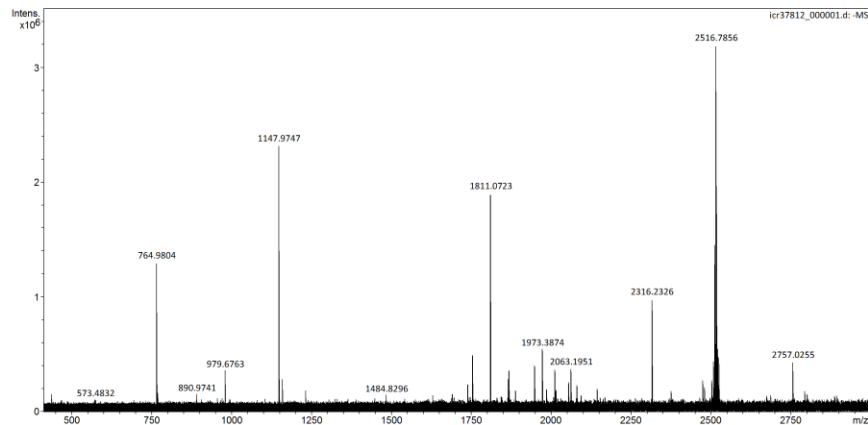
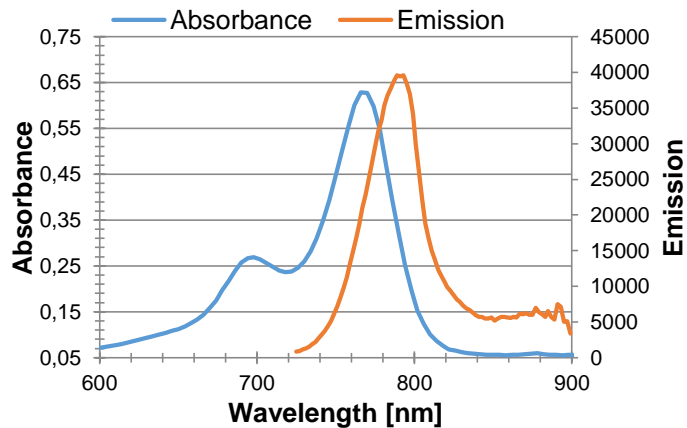


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3,64	n.a.	30,533	3,502	2,04	n.a.	BMB*
2	3,85	n.a.	2779,216	167,922	97,96	n.a.	BMB*
Total:			2809,749	171,424	100,00	0,000	





probe P13 in PBS (10 μM)



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3.67	n.a.	0,000	0,000	0,00	n.a.	Ru*
2	3.64	n.a.	45,258	5,571	10,29	n.a.	BM *
3	3.80	n.a.	827,727	48,545	89,71	n.a.	MB*
Total:			872,985	54,116	100,00	0,000	

