

Diphenyl-benzo[1,3]dioxole-4-carboxylic acid pentafluorophenyl ester : a convenient catechol precursor in the synthesis of siderophore vectors suitable for antibiotic Trojan horse strategies

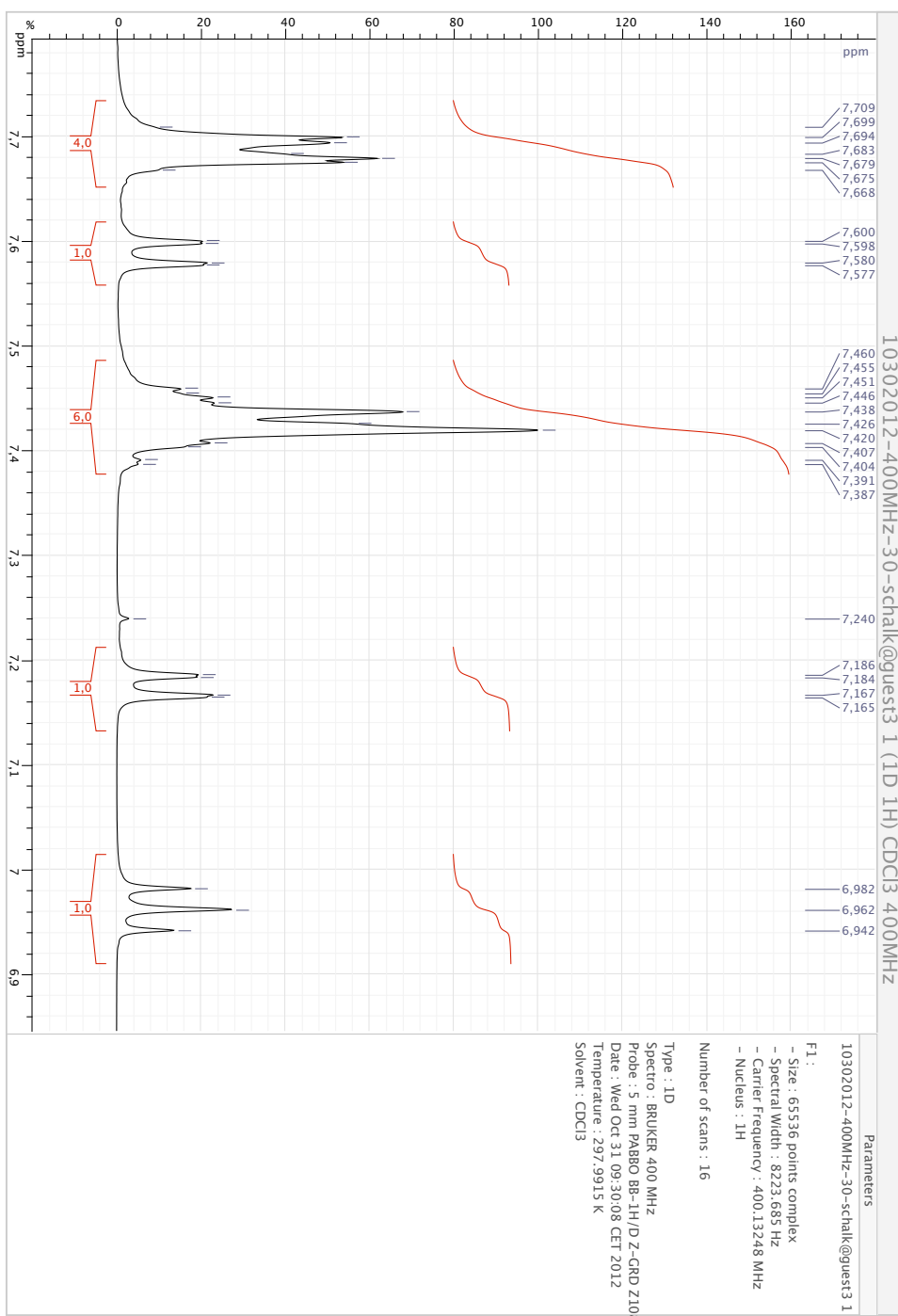
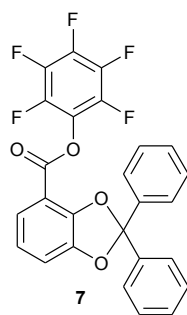
Etienne Baco, Françoise Hoegy, Isabelle J. Schalk and Gaëtan L. A. Mislin*

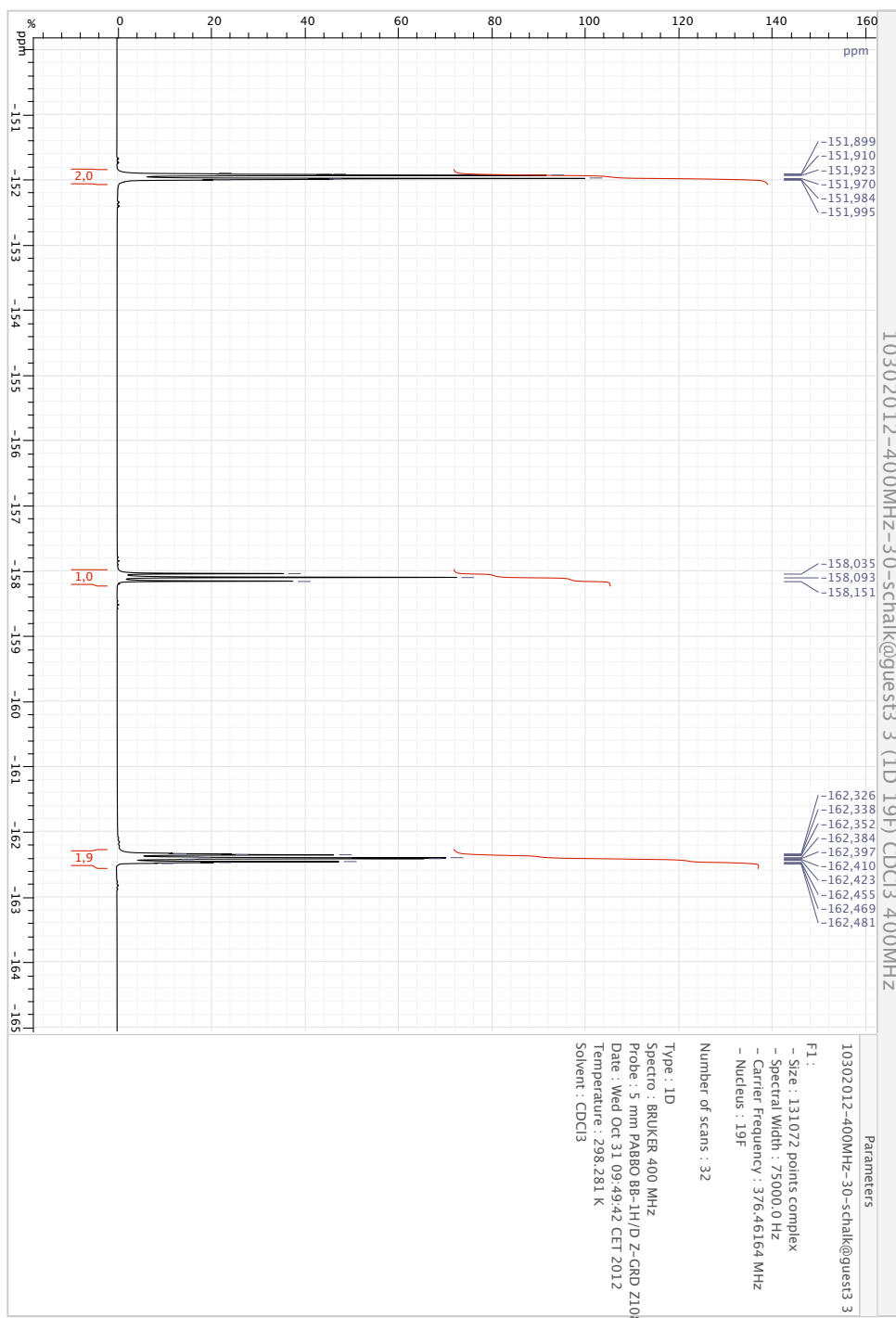
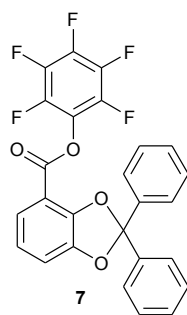
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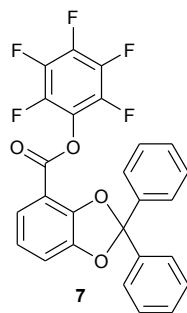
mislin@unistra.fr

SUPPORTING INFORMATIONS

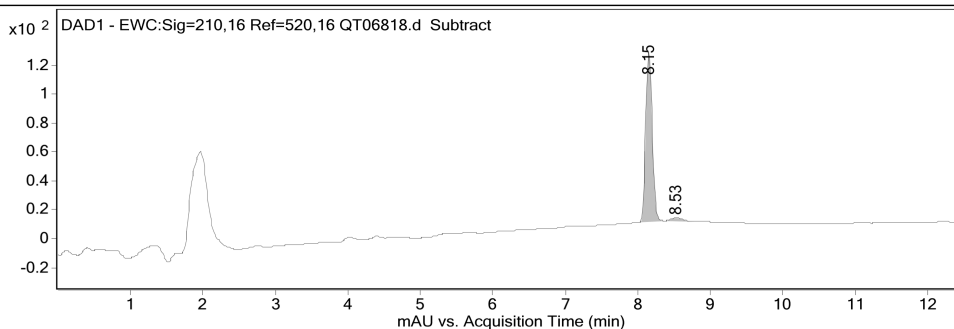
¹ H-NMR Spectrum of pentafluorophenylester 7	S1
¹⁹ F-NMR Spectrum of pentafluorophenylester 7	S2
LC-HRMS Spectrum of pentafluorophenylester 7	S3
¹ H-NMR Spectrum of bis-catechol chelator 1	S4
LC-HRMS Spectrum of bis-catechol chelator 1	S5
¹ H-NMR Spectrum of tris-catechol chelator 2	S6
LC-HRMS Spectrum of of tris-catechol chelator 2	S7





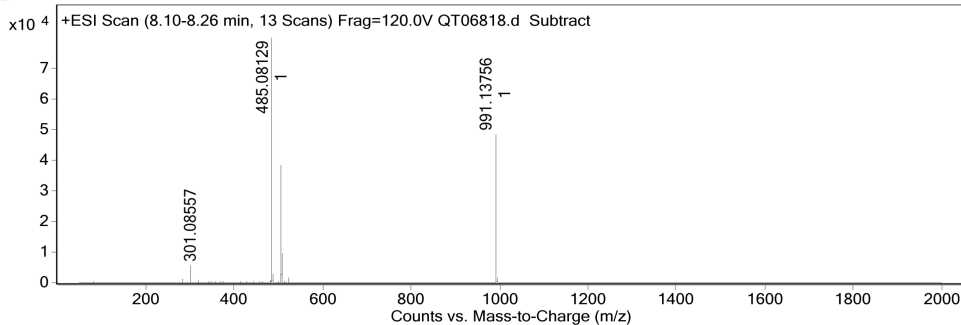


Qualitative Analysis Report



Start	RT	End	Height	Area	Area %	AreaSum%
8.03	8.15	8.38	118.3	736.973	100	96.71
8.38	8.53	8.78	2.2	25.043	3.4	3.29

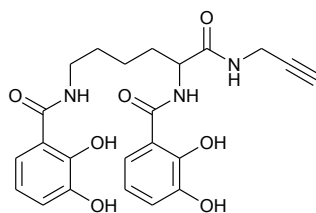
Spectrum Source: Peak (2) in "+" BPC(50.00000-1000.00000 [-39]) Scan"
 Fragmentor Voltage: 120
 Collision Energy: 0
 Ionization Mode: ESI



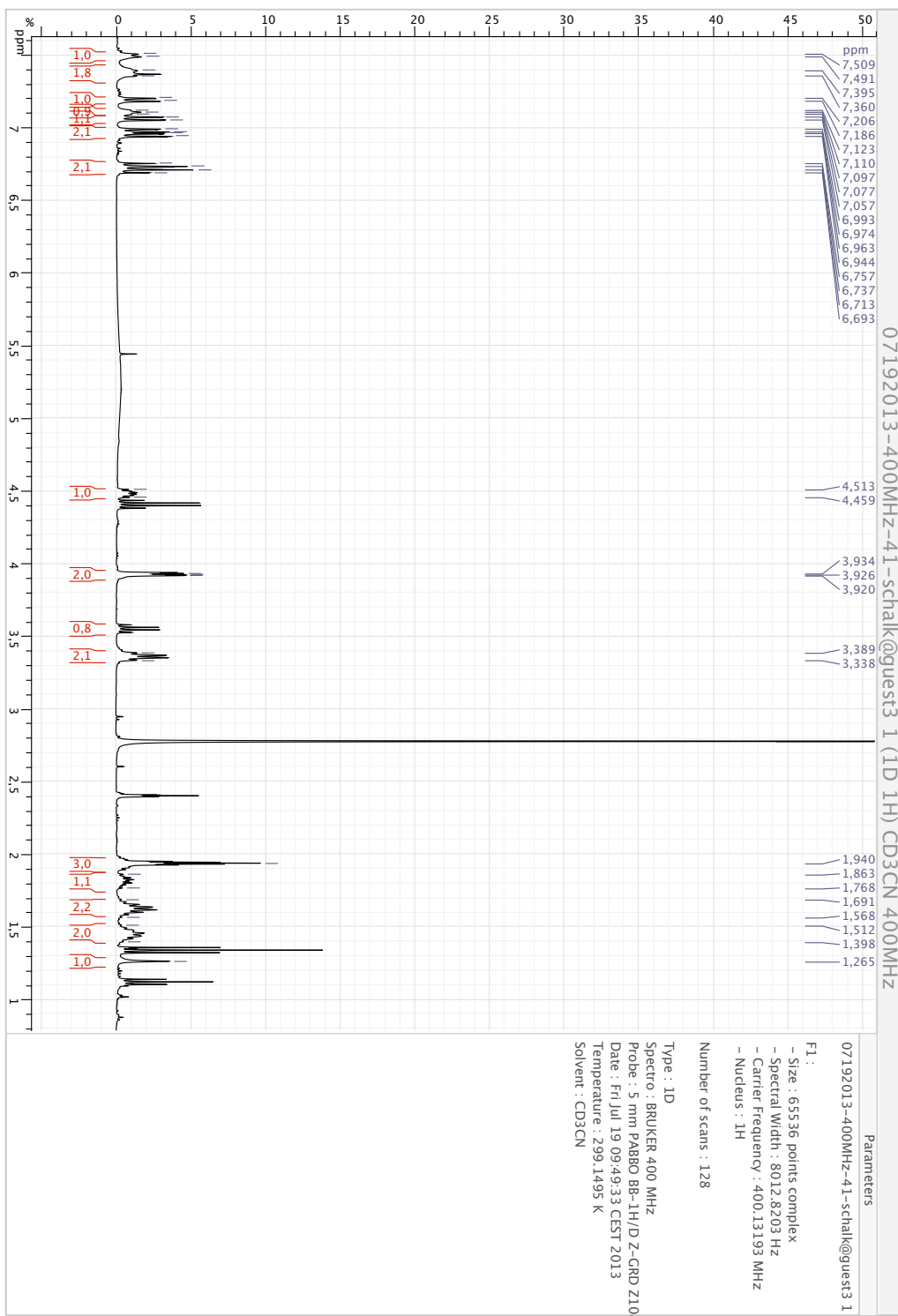
m/z	z	Abund	Formula	Ion
301.08557		5696.2		
485.08129	1	80237.1	C ₂₆ H ₁₄ F ₅ O ₄	(M+H) ⁺
486.08426	1	19975.2	C ₂₆ H ₁₄ F ₅ O ₄	(M+H) ⁺
507.06278	1	38410	C ₂₆ H ₁₃ F ₅ NaO ₄	(M+Na) ⁺
508.06582	1	9971.2	C ₂₆ H ₁₃ F ₅ NaO ₄	(M+Na) ⁺
991.13756	1	48553.1	C ₅₂ H ₂₆ F ₁₀ NaO ₈	(2M+Na) ⁺
992.14033	1	25083	C ₅₂ H ₂₆ F ₁₀ NaO ₈	(2M+Na) ⁺
993.14229	1	7284.4	C ₅₂ H ₂₆ F ₁₀ NaO ₈	(2M+Na) ⁺

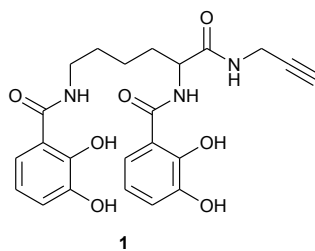
Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score
C ₂₃ H ₁₄ F ₆ O ₅		484.07401	484.07454	1.1	485.08129	C ₂₃ H ₁₅ F ₆ O ₅	99.2
C ₂₆ H ₁₃ F ₅ O ₄	TRUE	484.07401	484.0734	-1.26	485.08129	C ₂₆ H ₁₄ F ₅ O ₄	96.47
C ₂₀ H ₁₅ F ₇ O ₆		484.07401	484.07569	3.46	485.08129	C ₂₀ H ₁₆ F ₇ O ₆	93.44
C ₂₈ H ₁₄ F ₂ O ₆		484.07401	484.07584	3.79	485.08129	C ₂₈ H ₁₅ F ₂ O ₆	88.35
C ₂₉ H ₁₂ F ₄ O ₃		484.07401	484.07226	-3.62	485.08129	C ₂₉ H ₁₃ F ₄ O ₃	87.01
C ₃₁ H ₁₃ F ₅ O ₅		484.07401	484.0747	1.43	485.08129	C ₃₁ H ₁₄ F ₅ O ₅	85.85
C ₂₆ H ₁₃ F ₅ O ₄	TRUE	484.07355	484.0734	-0.31	507.06278	C ₂₆ H ₁₃ F ₅ NaO ₄	98.51
C ₂₃ H ₁₄ F ₆ O ₅		484.07355	484.07454	2.05	507.06278	C ₂₃ H ₁₄ F ₆ NaO ₅	98.21
C ₂₉ H ₁₂ F ₄ O ₃		484.07355	484.07226	-2.67	507.06278	C ₂₉ H ₁₂ F ₄ NaO ₃	91.52
C ₂₀ H ₁₅ F ₇ O ₆		484.07355	484.07569	4.41	507.06278	C ₂₀ H ₁₅ F ₇ NaO ₆	89.9
C ₂₈ H ₁₄ F ₂ O ₆		484.07355	484.07584	4.74	507.06278	C ₂₈ H ₁₄ F ₂ NaO ₆	88.69
C ₃₁ H ₁₃ F ₅ O ₅		484.07355	484.0747	2.38	507.06278	C ₃₁ H ₁₃ F ₅ NaO ₅	87.54
C ₅₂ H ₂₆ F ₁₀ O ₈	TRUE	968.14826	968.1468	-1.51	991.13756	C ₅₂ H ₂₆ F ₁₀ NaO ₈	95.95
C ₅₄ H ₂₇ F ₇ O ₁₀		968.14826	968.14924	1.02	991.13756	C ₅₄ H ₂₇ F ₇ NaO ₁₀	94.6
C ₅₇ H ₂₆ F ₆ O ₉		968.14826	968.1481	-0.16	991.13756	C ₅₇ H ₂₆ F ₆ NaO ₉	91.82
C ₅₅ H ₂₅ F ₉ O ₇		968.14826	968.14566	-2.69	991.13756	C ₅₅ H ₂₅ F ₉ NaO ₇	90.63
C ₆₀ H ₂₅ F ₅ O ₈		968.14826	968.14696	-1.34	991.13756	C ₆₀ H ₂₅ F ₅ NaO ₈	87.19

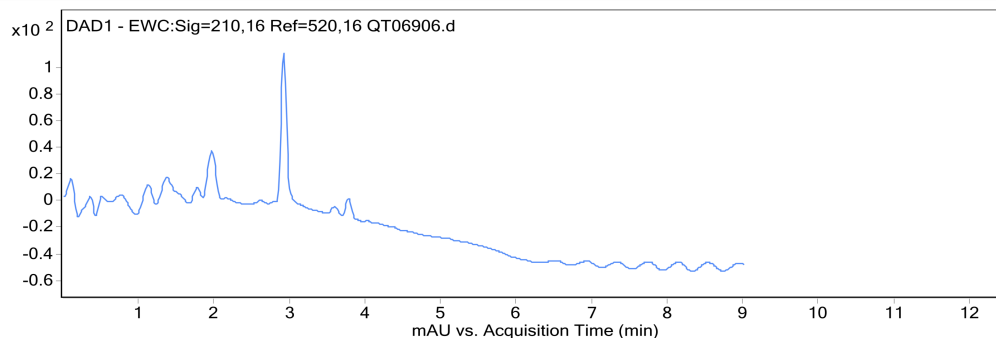


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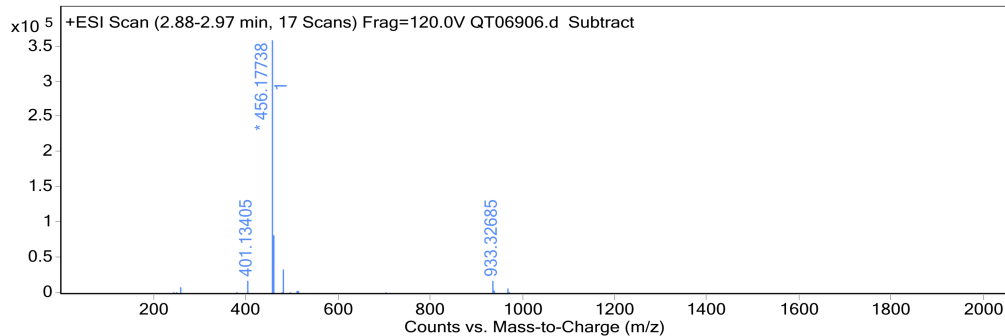




Qualitative Analysis Report



Spectrum Source: Peak (4) in "+ BPC(50.00000-1000.00000 [-41]) Scan"
 Fragmentor Voltage: 120
 Collision Energy: 0
 Ionization Mode: ESI

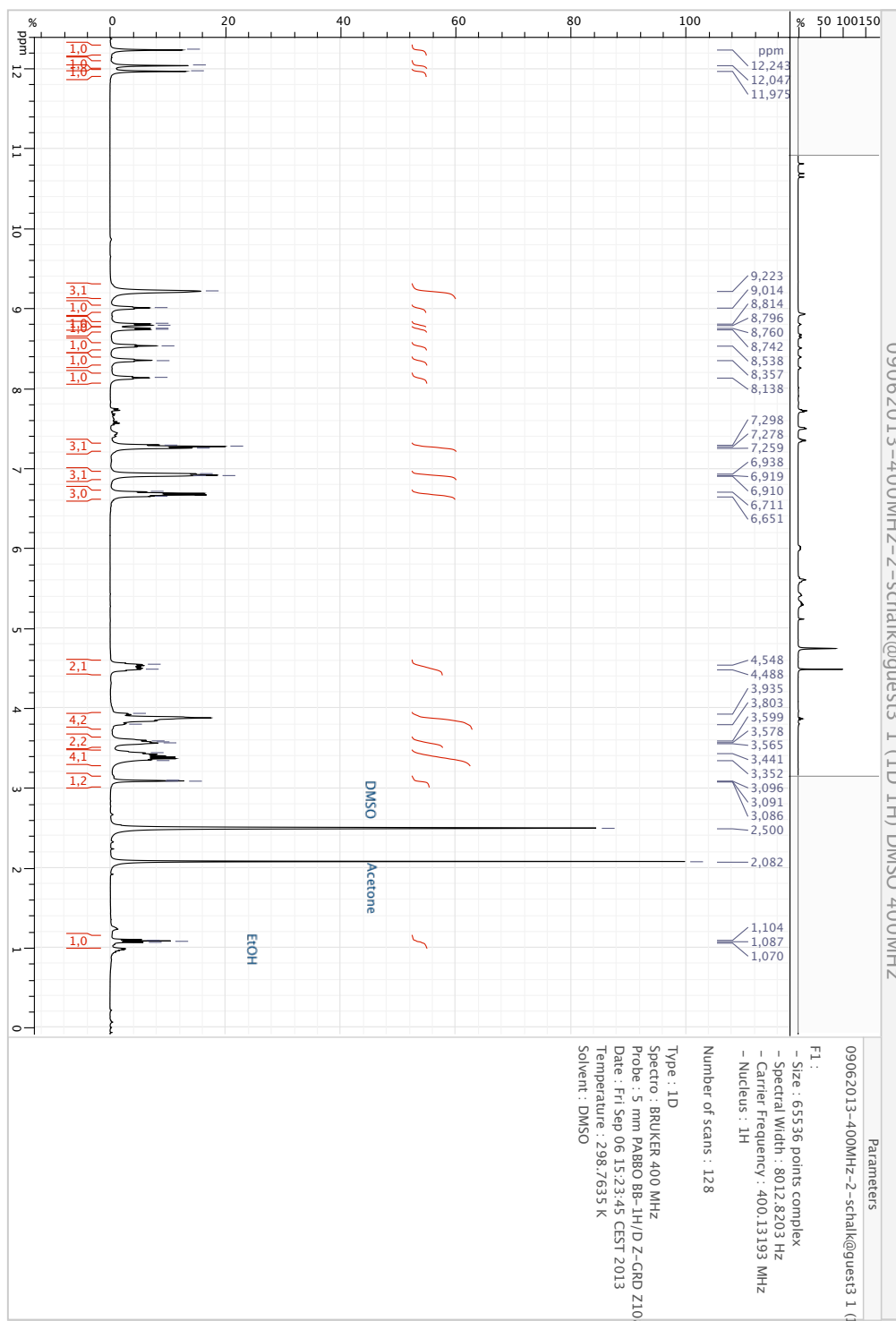
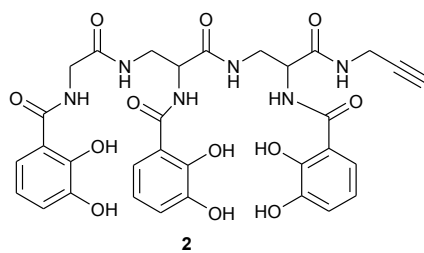


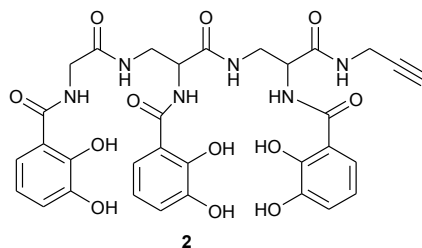
Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
401.13405		18534.2		
456.17738	1	359223.9	C ₂₄ H ₂₂ N ₇ O ₃	(M+H) ⁺
457.17973	1	83846.8	C ₂₄ H ₂₂ N ₇ O ₃	(M+H) ⁺
478.15849		33277.5		
933.32685		18580.5		

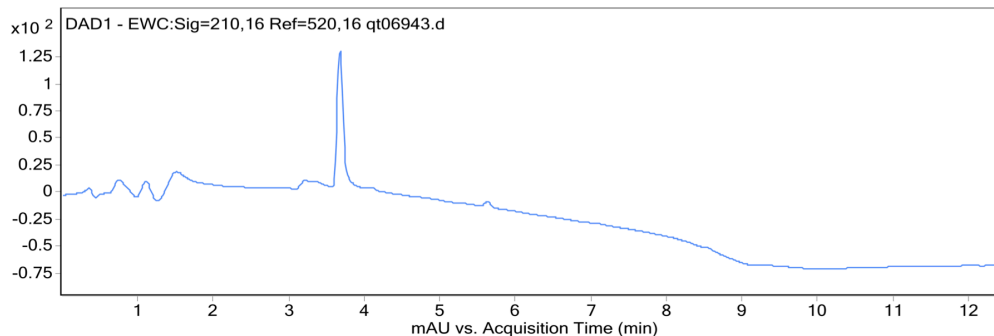
Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	<i>Mz</i>	Ion Species	Score
C ₂₄ H ₂₁ N ₇ O ₃		455.1701	455.17059	1.08	456.17738	C ₂₄ H ₂₂ N ₇ O ₃	97.78
C ₂₃ H ₂₅ N ₃ O ₇	TRUE	455.17009	455.16925	-1.85	456.17738	C ₂₃ H ₂₆ N ₃ O ₇	97.26

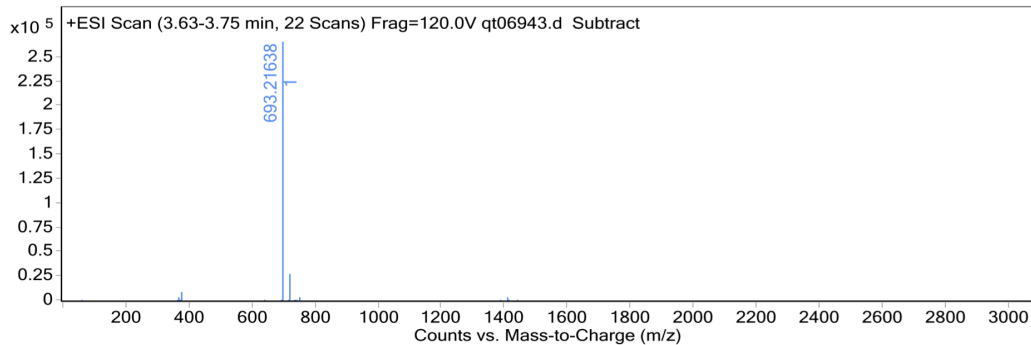




Qualitative Analysis Report



Spectrum Source Peak (1) in "+ BPC(50.00000-1000.00000 [-41]) Scan"
Fragmentor Voltage 120
Collision Energy 0
Ionization Mode ESI



Peak List

m/z	z	Abund	Formula	Ion
693.21638	1	269453.7	C33 H29 N10 O8	(M+H)+
694.21876	1	90545.4	C33 H29 N10 O8	(M+H)+
695.22083	1	18788.2	C33 H29 N10 O8	(M+H)+
715.19718		27962.6		

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score
C33 H28 N10 O8		692.20908	692.20916	0.11	693.21638	C33 H29 N10 O8	98.64
C32 H32 N6 O12	TRUE	692.20907	692.20782	-1.81	693.21638	C32 H33 N6 O12	96.95
C34 H24 N14 O4		692.20909	692.2105	2.03	693.21638	C34 H25 N14 O4	95.24
C36 H36 O14		692.20906	692.21051	2.09	693.21638	C36 H37 O14	95.07
C21 H32 N12 O15		692.2091	692.21101	2.76	693.21638	C21 H33 N12 O15	94.01
C49 H28 N2 O3		692.20906	692.20999	1.34	693.21638	C49 H29 N2 O3	89.83