Synthesis and antibiotic activity of oxazolidinone-catechol conjugates against *Pseudomonas aeruginosa*

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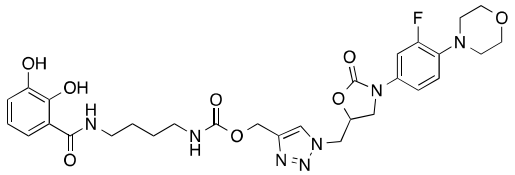
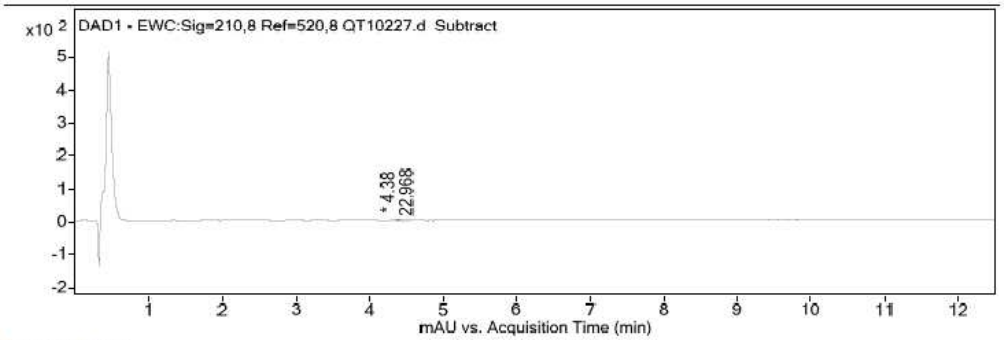
SUPPORTING INFORMATIONS



10



Integration Peak List

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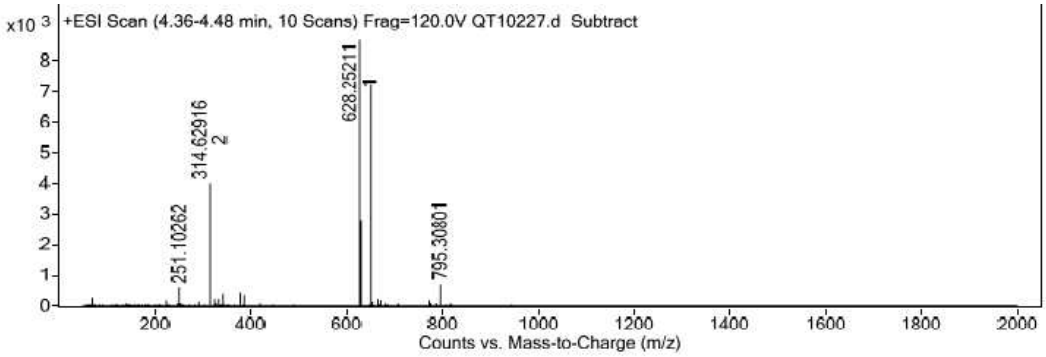
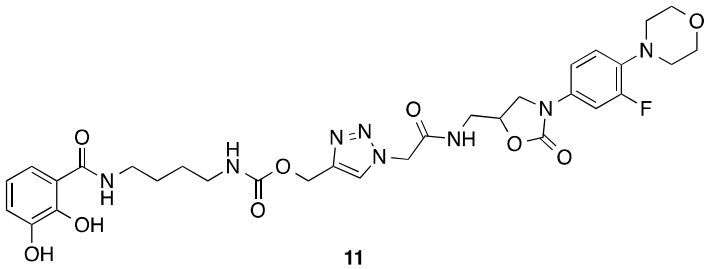


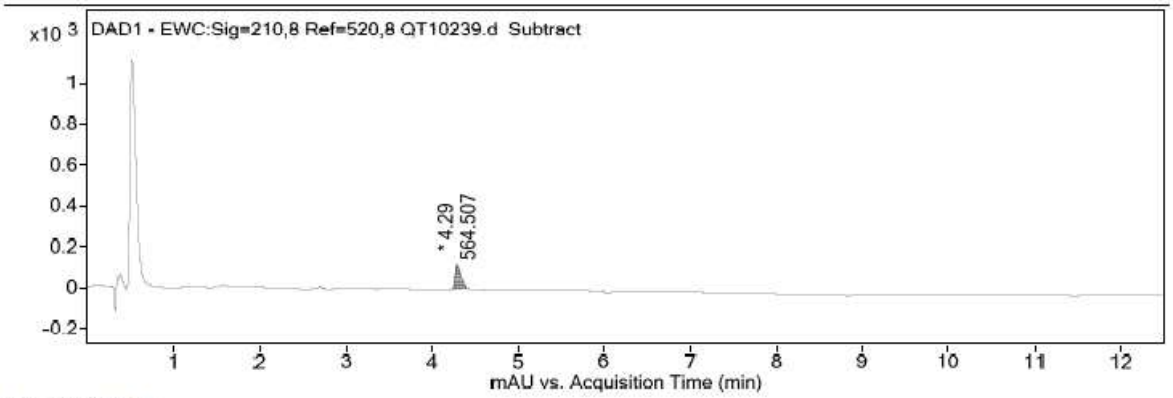
Peak List

m/z	z	Abund	Formula	Ion
251.10262		599.9		
314.62916	2	4015.2	C29 H36 F N7 O8	(M+2H)+2
315.13169	2	1318.6	C29 H36 F N7 O8	(M+2H)+2
628.25211	1	8727.4	C29 H35 F N7 O8	(M+H)+
629.25521	1	2791.7	C29 H35 F N7 O8	(M+H)+
630.25852	1	529.3	C29 H35 F N7 O8	(M+H)+
650.23447	1	7248.2	C29 H34 F N7 Na O8	(M+Na)+
651.23735	1	2298.3	C29 H34 F N7 Na O8	(M+Na)+
652.23991	1	525.6	C29 H34 F N7 Na O8	(M+Na)+
795.30801		719		

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score
C29 H34 F N7 O8	TRUE	627.24525	627.24529	0.07	650.23447	C29 H34 F N7 Na O8	98.72
C25 H39 F2 N3 O13		627.24524	627.24509	-0.23	650.23447	C25 H39 F2 N3 Na O13	98.24
C26 H35 F2 N7 O9		627.24525	627.24643	1.89	650.23447	C26 H35 F2 N7 Na O9	97.78
C28 H38 F N3 O12		627.24524	627.24395	-2.05	650.23447	C28 H38 F N3 Na O12	97.37
C34 H36 F3 N O7		627.24524	627.24439	-1.35	650.23447	C34 H36 F3 N Na O7	94.49
C27 H36 F3 N7 O5 S		627.24525	627.24507	-0.29	650.23447	C27 H36 F3 N7 Na O5 S	94.19
C32 H33 N7 O7		627.24525	627.24415	-1.75	650.23447	C32 H33 N7 Na O7	94.09
C20 H37 N9 O14		627.24526	627.246	1.18	650.23447	C20 H37 N9 Na O14	93.37
C22 H40 F3 N3 O14		627.24524	627.24624	1.59	650.23447	C22 H40 F3 N3 Na O14	92.88
C35 H32 F3 N5 O3		627.24524	627.24572	0.77	650.23447	C35 H32 F3 N5 Na O3	91.95
C29 H34 F N7 O8	TRUE	627.24484	627.24529	0.72	628.25211	C29 H35 F N7 O8	98.57
C28 H38 F N3 O12		627.24483	627.24395	-1.4	628.25211	C28 H39 F N3 O12	98.38
C25 H39 F2 N3 O13		627.24483	627.24509	0.42	628.25211	C25 H40 F2 N3 O13	98.02
C26 H35 F2 N7 O9		627.24484	627.24643	2.54	628.25211	C26 H36 F2 N7 O9	96.34
C34 H36 F3 N O7		627.24483	627.24439	-0.7	628.25211	C34 H37 F3 N O7	95.53
C32 H33 N7 O7		627.24484	627.24415	-1.1	628.25211	C32 H34 N7 O7	95.11
C31 H37 N3 O11		627.24483	627.24281	-3.22	628.25211	C31 H38 N3 O11	92.73
C27 H36 F3 N7 O5 S		627.24484	627.24507	0.36	628.25211	C27 H37 F3 N7 O5 S	92.63
C20 H37 N9 O14		627.24485	627.246	1.83	628.25211	C20 H38 N9 O14	91.79
C35 H32 F3 N5 O3		627.24483	627.24572	1.42	628.25211	C35 H33 F3 N5 O3	91.57
C28 H38 F N3 O12		627.24383	627.24395	0.19	314.62916	C28 H40 F N3 O12	98.66
C31 H37 N3 O11		627.24383	627.24281	-1.63	314.62916	C31 H39 N3 O11	97.1
C29 H34 F N7 O8	TRUE	627.24384	627.24529	2.3	314.62916	C29 H36 F N7 O8	96.51
C34 H36 F3 N O7		627.24383	627.24439	0.89	314.62916	C34 H38 F3 N O7	95.75
C25 H39 F2 N3 O13		627.24384	627.24509	2.01	314.62916	C25 H41 F2 N3 O13	95.53
C32 H33 N7 O7		627.24384	627.24415	0.48	314.62916	C32 H35 N7 O7	95.47
C30 H32 F3 N7 O5		627.24384	627.2417	-3.41	314.62916	C30 H34 F3 N7 O5	94.1
C26 H35 F2 N7 O9		627.24385	627.24643	4.12	314.62916	C26 H37 F2 N7 O9	93.47
C30 H35 F2 N7 O4 S		627.24385	627.24393	0.13	314.62916	C30 H37 F2 N7 O4 S	92.78
C27 H36 F3 N7 O5 S		627.24385	627.24507	1.95	314.62916	C27 H38 F3 N7 O5 S	92.5



11



Integration Peak List

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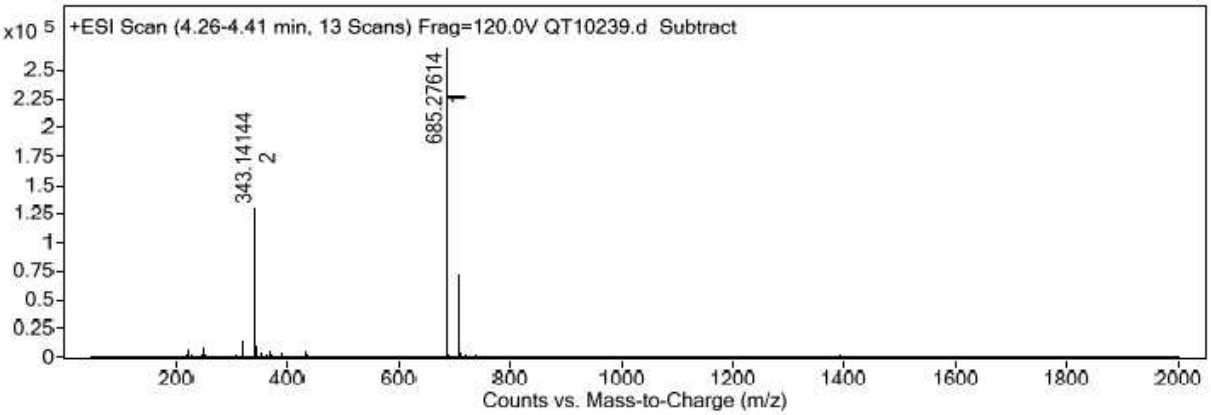
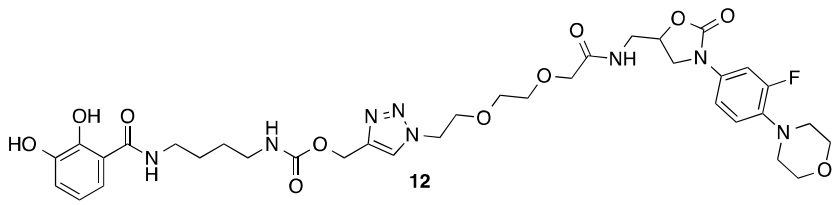


Peak List

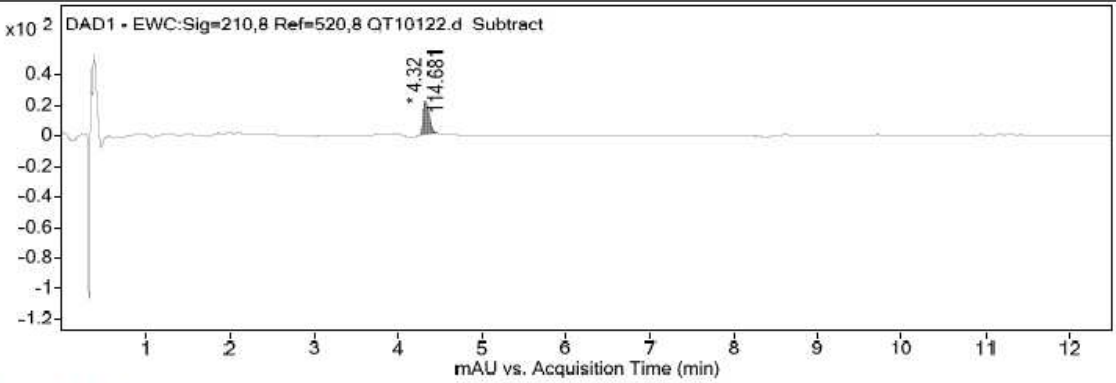
m/z	z	Abund	Formula	Ion
343.14144	2	132738.1		
343.64271	2	43830.9		
685.27614	1	278427.4	C31 H38 F N8 O9	(M+H)+
686.27865	1	89572.3	C31 H38 F N8 O9	(M+H)+
687.2807	1	15803.7	C31 H38 F N8 O9	(M+H)+
707.25736	1	71602.8		
708.26037	1	21754.9		

Formula Calculator Results

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score
C25 H39 F3 N8 O11		684.26885	684.26904	0.28	685.27614	C25 H40 F3 N8 O11	98.53
C28 H38 F2 N8 O10		684.26885	684.2679	-1.39	685.27614	C28 H39 F2 N8 O10	97.46
C26 H44 N4 O17		684.26884	684.27015	1.91	685.27614	C26 H45 N4 O17	94.77
C24 H43 F3 N4 O15		684.26884	684.2677	-1.66	685.27614	C24 H44 F3 N4 O15	94.26
C22 H40 N10 O15		684.26886	684.26746	-2.04	685.27614	C22 H41 N10 O15	93.73
C32 H42 F2 N2 O12		684.26883	684.27058	2.55	685.27614	C32 H43 F2 N2 O12	92.55
C35 H41 F N2 O11		684.26883	684.26944	0.88	685.27614	C35 H42 F N2 O11	92.07
C27 H42 F2 N4 O14		684.26884	684.26656	-3.33	685.27614	C27 H43 F2 N4 O14	91.99
C31 H37 F N8 O9	TRUE	684.26885	684.26675	-3.06	685.27614	C31 H38 F N8 O9	91.03
C27 H40 N8 O13		684.26885	684.27148	3.85	685.27614	C27 H41 N8 O13	90.58



12



Integration Peak List

Start	RT	End	Height	Area	Area %	AreaSum%
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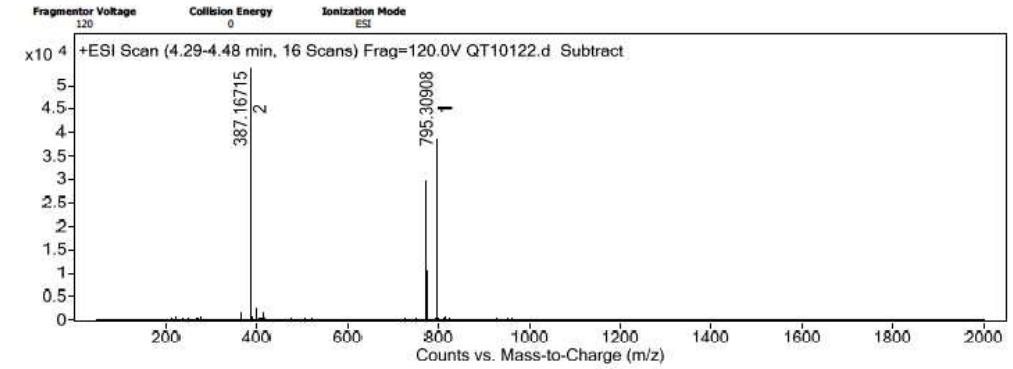
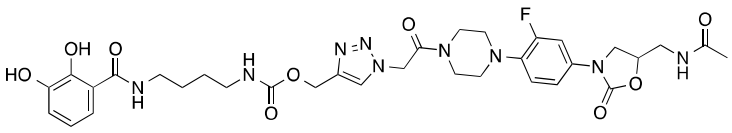


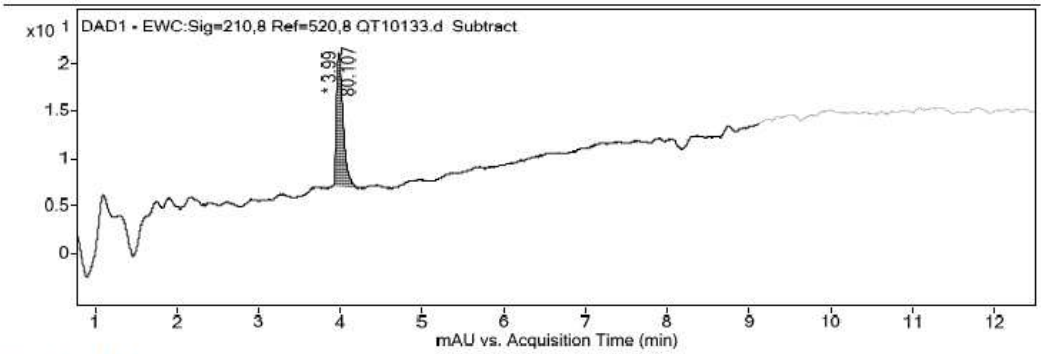
Peak List

m/z	z	Abund	Formula	Ion
387.16715	2	55535.7	C35 H47 F N8 O11	(M+2H)+2
387.66821	2	21454.3	C35 H47 F N8 O11	(M+2H)+2
388.16931	2	5154	C35 H47 F N8 O11	(M+2H)+2
773.32708	1	29648.3	C35 H46 F N8 O11	(M+H)+
774.32975	1	10636.7	C35 H46 F N8 O11	(M+H)+
795.30908	1	39140.6	C35 H45 F N8 Na O11	(M+Na)+
796.31159	1	14080.5	C35 H45 F N8 Na O11	(M+Na)+
797.31355	1	3079.4	C35 H45 F N8 Na O11	(M+Na)+

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score
C32 H46 F2 N8 O12		772.31971	772.32033	0.8	387.16715	C32 H48 F2 N8 O12	99.34
C35 H45 F N8 O11	TRUE	772.31971	772.31918	-0.68	387.16715	C35 H47 F N8 O11	98.18
C27 H44 N14 O13		772.31973	772.32123	1.93	387.16715	C27 H46 N14 O13	96.85
C30 H45 F5 N8 O10		772.31971	772.31788	-2.37	387.16715	C30 H47 F5 N8 O10	96.84
C28 H42 F2 N14 O10		772.31973	772.31764	-2.71	387.16715	C28 H44 F2 N14 O10	96.5
C29 H47 F3 N8 O13		772.31971	772.32147	2.27	387.16715	C29 H49 F3 N8 O13	96.14
C25 H43 F3 N14 O11		772.31974	772.31878	-1.24	387.16715	C25 H45 F3 N14 O11	94.79
C26 H48 N10 O17		772.31972	772.31989	0.22	387.16715	C26 H50 N10 O17	94.63
C38 H44 N8 O10		772.31971	772.31804	-2.16	387.16715	C38 H46 N8 O10	93.36
C27 H46 F2 N10 O14		772.31972	772.3163	-4.43	387.16715	C27 H48 F2 N10 O14	89.9
C32 H46 F2 N8 O12		772.31979	772.32033	0.7	773.32708	C32 H47 F2 N8 O12	98.31
C26 H48 N10 O17		772.3198	772.31989	0.12	773.32708	C26 H49 N10 O17	97.78
C27 H44 N14 O13		772.31981	772.32123	1.84	773.32708	C27 H45 N14 O13	97.63
C25 H43 F3 N14 O11		772.31981	772.31878	-1.33	773.32708	C25 H44 F3 N14 O11	97.54
C29 H47 F3 N8 O13		772.31979	772.32147	2.17	773.32708	C29 H48 F3 N8 O13	96.75
C30 H45 F5 N8 O10		772.31979	772.31788	-2.47	773.32708	C30 H46 F5 N8 O10	96.15
C28 H42 F2 N14 O10		772.31981	772.31764	-2.81	773.32708	C28 H43 F2 N14 O10	95.3
C35 H45 F N8 O11	TRUE	772.31979	772.31918	-0.78	773.32708	C35 H46 F N8 O11	94.8
C22 H44 F4 N14 O12		772.31981	772.31993	0.14	773.32708	C22 H45 F4 N14 O12	94.07
C25 H52 N6 O21		772.31979	772.31855	-1.6	773.32708	C25 H53 N6 O21	92.35
C32 H46 F2 N8 O12		772.31984	772.32033	0.62	795.30908	C32 H46 F2 N8 Na O12	98.28
C27 H44 N14 O13		772.31986	772.32123	1.77	795.30908	C27 H44 N14 Na O13	97.73
C26 H48 N10 O17		772.31985	772.31989	0.05	795.30908	C26 H48 N10 Na O17	97.49
C25 H43 F3 N14 O11		772.31987	772.31878	-1.4	795.30908	C25 H43 F3 N14 Na O11	97.36
C29 H47 F3 N8 O13		772.31984	772.32147	2.1	795.30908	C29 H47 F3 N8 Na O13	96.85
C30 H45 F5 N8 O10		772.31984	772.31788	-2.54	795.30908	C30 H45 F5 N8 Na O10	96.01
C28 H42 F2 N14 O10		772.31986	772.31764	-2.88	795.30908	C28 H42 F2 N14 Na O10	95.22
C35 H45 F N8 O11	TRUE	772.31984	772.31918	-0.85	795.30908	C35 H45 F N8 Na O11	94.7
C22 H44 F4 N14 O12		772.31987	772.31993	0.07	795.30908	C22 H44 F4 N14 Na O12	93.92
C25 H52 N6 O21		772.31984	772.31855	-1.67	795.30908	C25 H52 N6 Na O21	91.84



13



Integration Peak List

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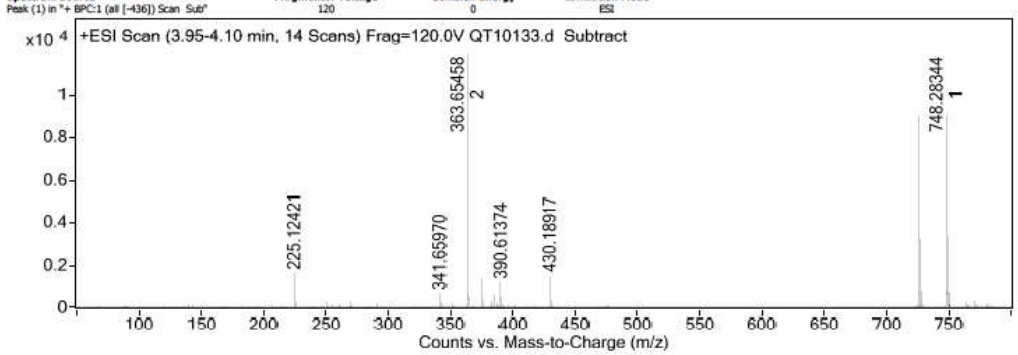
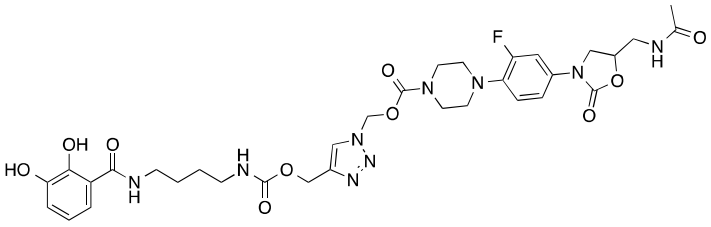


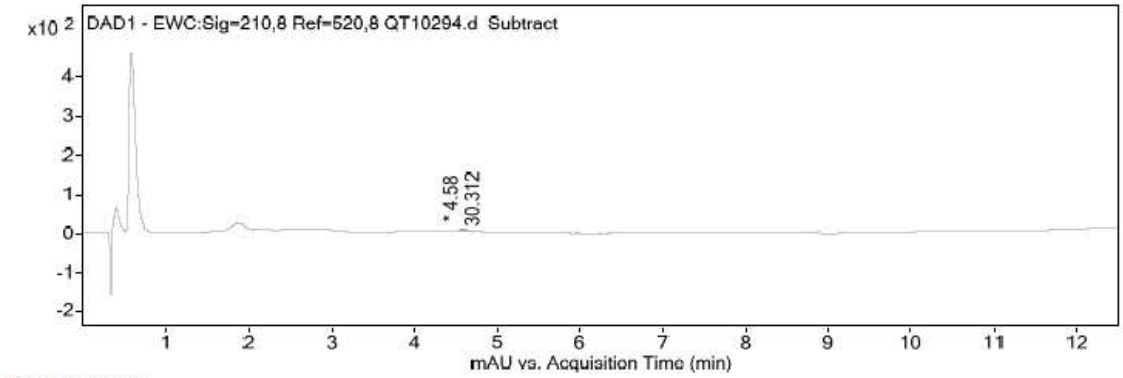
Peak List

m/z	z	Abund	Formula	Ion
225.12421		1677.5		
363.65458	2	11999.5	C33 H42 F N9 O9	(M+2H)+2
364.15616	2	4650.4	C33 H42 F N9 O9	(M+2H)+2
374.64536	2	1356.6		
390.61374		1170.1		
430.18917		1473		
726.30169	1	9235	C33 H41 F N9 O9	(M+H)+
727.30401	1	3231	C33 H41 F N9 O9	(M+H)+
748.28344	1	9081.8	C33 H40 F N9 Na O9	(M+Na)+
749.28719	1	3341.9	C33 H40 F N9 Na O9	(M+Na)+

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score
C33 H40 F N9 O9	TRUE	725.29426	725.2933	-1.33	748.28344	C33 H40 F N9 Na O9	97.75
C32 H47 N5 O12 S		725.29426	725.29419	-0.09	748.28344	C32 H47 N5 Na O12 S	95.14
C40 H43 N3 O10		725.29425	725.29484	0.82	748.28344	C40 H43 N3 Na O10	94.63
C37 H44 F N3 O11		725.29425	725.29599	2.4	748.28344	C37 H44 F N3 Na O11	94.33
C32 H44 F N5 O13		725.29425	725.29196	-3.16	748.28344	C32 H44 F N5 Na O13	93.98
C33 H43 N9 O8 S		725.29427	725.29553	1.74	748.28344	C33 H43 N9 Na O8 S	93.43
C29 H48 F N5 O13 S		725.29426	725.29534	1.48	748.28344	C29 H48 F N5 Na O13 S	93.39
C28 H52 F N O17 S		725.29425	725.294	-0.34	748.28344	C28 H52 F N Na O17 S	92.75
C36 H39 N9 O8		725.29426	725.29216	-2.9	748.28344	C36 H39 N9 Na O8	92.35
C31 H51 N O16 S		725.29425	725.29286	-1.92	748.28344	C31 H51 N Na O16 S	92.26
C33 H40 F N9 O9	TRUE	725.29439	725.2933	-1.5	726.30169	C33 H41 F N9 O9	96.84
C32 H47 N5 O12 S		725.29439	725.29419	-0.27	726.30169	C32 H48 N5 O12 S	94.81
C29 H48 F N5 O13 S		725.29439	725.29534	1.31	726.30169	C29 H49 F N5 O13 S	94.03
C28 H47 N5 O17		725.29438	725.2967	3.19	726.30169	C28 H48 N5 O17	93.72
C37 H44 F N3 O11		725.29438	725.29599	2.22	726.30169	C37 H45 F N3 O11	93.39
C28 H52 F N O17 S		725.29438	725.294	-0.52	726.30169	C28 H53 F N O17 S	93.32
C23 H47 N7 O19		725.29439	725.29267	-2.37	726.30169	C23 H48 N7 O19	93.1
C32 H44 F N5 O13		725.29438	725.29196	-3.33	726.30169	C32 H45 F N5 O13	93.09
C40 H43 N3 O10		725.29438	725.29484	0.65	726.30169	C40 H44 N3 O10	93.04
C33 H43 N9 O8 S		725.2944	725.29553	1.56	726.30169	C33 H44 N9 O8 S	93.02
C33 H40 F N9 O9	TRUE	725.29462	725.2933	-1.81	363.65458	C33 H42 F N9 O9	98.75
C37 H44 F N3 O11		725.2946	725.29599	1.92	363.65458	C37 H46 F N3 O11	97.84
C40 H43 N3 O10		725.2946	725.29484	0.34	363.65458	C40 H45 N3 O10	97.21
C32 H44 F N5 O13		725.2946	725.29196	-3.64	363.65458	C32 H46 F N5 O13	95.39
C36 H39 N9 O8		725.29462	725.29216	-3.39	363.65458	C36 H41 N9 O8	95.09
C33 H43 N9 O8 S		725.29462	725.29553	1.25	363.65458	C33 H45 N9 O8 S	95.05
C32 H47 N5 O12 S		725.29461	725.29419	-0.58	363.65458	C32 H49 N5 O12 S	94.74
C28 H47 N5 O17		725.29461	725.2967	2.88	363.65458	C28 H49 N5 O17	94.57
C41 H39 N7 O6		725.29461	725.29618	2.17	363.65458	C41 H41 N7 O6	94.01
C38 H40 F N7 O7		725.29461	725.29732	3.75	363.65458	C38 H42 F N7 O7	93.52



14



Integration Peak List

Start	RT	End	Height	Area	Area %	AreaSum%
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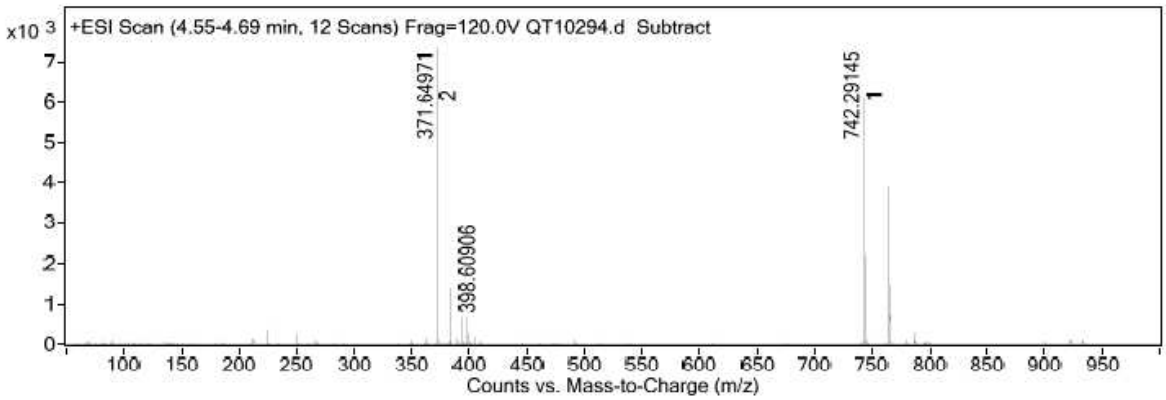
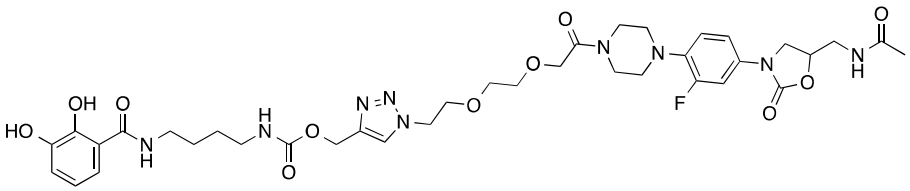


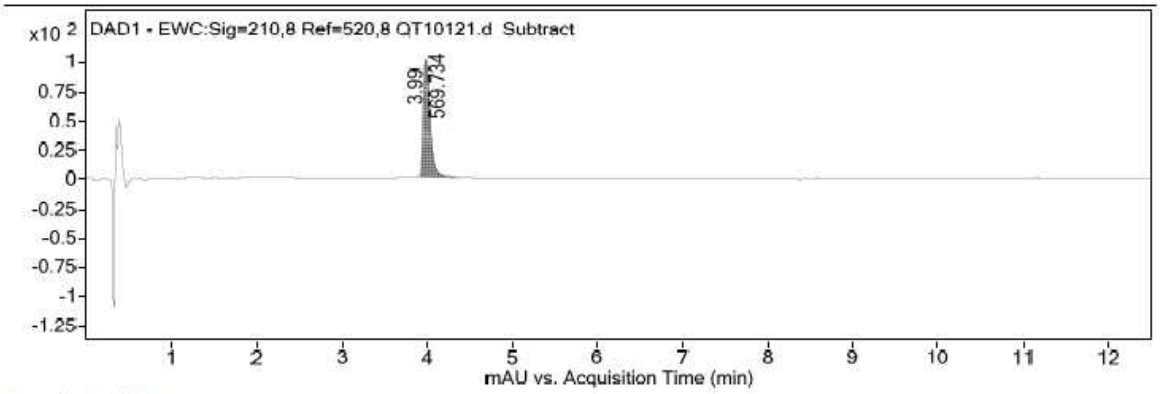
Peak List

m/z	z	Abund	Formula	Ion
371.64971	2	7456.7	C33 H40 F N9 O10	(M+2H)+2
372.15055	2	2811.6	C33 H40 F N9 O10	(M+2H)+2
372.65214	2	671.7	C33 H40 F N9 O10	(M+2H)+2
382.63973	2	1391.8		
393.63117		678.9		
398.60906		673.9		
742.29145	1	6173.7	C33 H40 F N9 O10	(M+H)+
743.29488	1	2218.4	C33 H40 F N9 O10	(M+H)+
764.27334	1	3903.5		
765.27667	1	1486.5		

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score	DBE
C28 H40 F N11 O12		741.28421	741.28419	-0.02	742.29145	C28 H41 F N11 O12	98.08	14
C29 H36 F N15 O8		741.28422	741.28553	1.77	742.29145	C29 H37 F N15 O8	96.02	19
C32 H44 F N5 O14		741.28419	741.28688	3.63	742.29145	C32 H45 F N5 O14	91.11	13
C29 H36 F N15 O8		741.28484	741.28553	0.94	371.64971	C29 H38 F N15 O8	98.92	19
C28 H40 F N11 O12		741.28482	741.28419	-0.85	371.64971	C28 H42 F N11 O12	97.78	14
C32 H44 F N5 O14		741.2848	741.28688	2.8	371.64971	C32 H46 F N5 O14	95.68	13
C33 H40 F N9 O10	TRUE	741.28481	741.28822	4.59	371.64971	C33 H42 F N9 O10	91.92	18
C44 H40 F N3 O7		741.2848	741.28503	0.32	371.64971	C44 H42 F N3 O7	88.68	26
C40 H36 F N9 O5		741.28481	741.28234	-3.33	371.64971	C40 H38 F N9 O5	88.42	27
C41 H32 F N13 O		741.28482	741.28368	-1.54	371.64971	C41 H34 F N13 O	88.41	32
C45 H36 F N7 O3		741.2848	741.28637	2.11	371.64971	C45 H38 F N7 O3	84.48	31



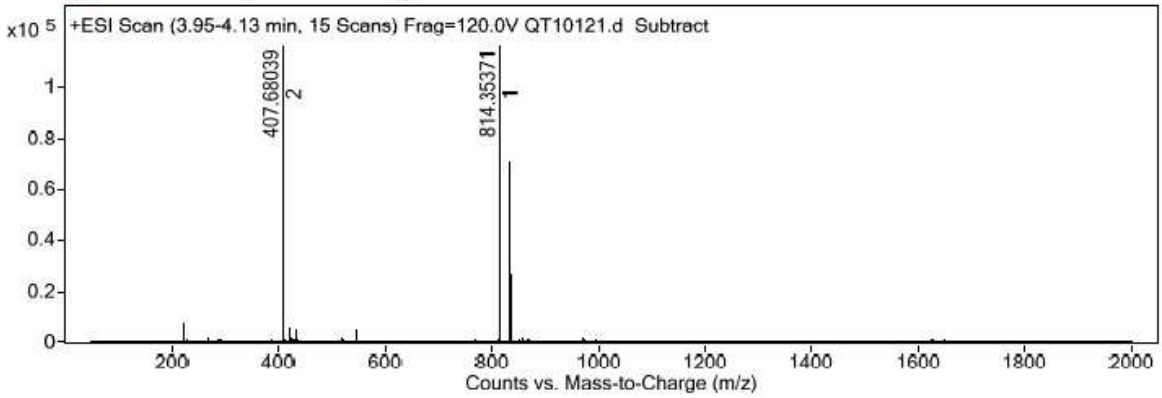
15



Integration Peak List

Start	RT	End	Height	Area	Area %	AreaSum%
3.9	3.99	4.43	100.94	569.734	100	100

Fragmentor Voltage 120 **Collision Energy** 0 **Ionization Mode** ESI



Peak List

m/z	z	Abund	Formula	Ion
407.68039	2	138819.7	C37 H50 F N9 O11	(M+2H)+2
408.18153	2	55905.3	C37 H50 F N9 O11	(M+2H)+2
408.68245	2	13137.9	C37 H50 F N9 O11	(M+2H)+2
814.35371	1	116508.2	C37 H49 F N9 O11	(M+H)+
815.35628	1	44332.6	C37 H49 F N9 O11	(M+H)+
816.35825	1	9355.6	C37 H49 F N9 O11	(M+H)+
836.33545	1	71999		
837.33807	1	27262		

Formula	Best	Mass	Tgt Mass	Diff (ppm)	Mz	Ion Species	Score
C34 H49 F2 N9 O12		813.34619	813.34687	0.84	407.68039	C34 H51 F2 N9 O12	99.26
C33 H53 F2 N5 O16		813.34618	813.34554	-0.79	407.68039	C33 H55 F2 N5 O16	98.76
C37 H48 F N9 O11	TRUE	813.34619	813.34573	-0.56	407.68039	C37 H50 F N9 O11	98.45
C29 H47 N15 O13		813.34622	813.34778	1.92	407.68039	C29 H49 N15 O13	98.04
C27 H46 F3 N15 O11		813.34622	813.34533	-1.09	407.68039	C27 H48 F3 N15 O11	97.97
C28 H51 N11 O17		813.3462	813.34644	0.29	407.68039	C28 H53 N11 O17	97.86
C32 H48 F5 N9 O10		813.34619	813.34443	-2.17	407.68039	C32 H50 F5 N9 O10	97.82
C30 H54 F3 N5 O17		813.34618	813.34668	0.62	407.68039	C30 H56 F3 N5 O17	97.5
C30 H45 F2 N15 O10		813.34622	813.34419	-2.49	407.68039	C30 H47 F2 N15 O10	97.48
C31 H50 F3 N9 O13		813.34619	813.34802	2.24	407.68039	C31 H52 F3 N9 O13	97.37
C34 H49 F2 N9 O12		813.34641	813.34687	0.57	814.35371	C34 H50 F2 N9 O12	98.6
C28 H51 N11 O17		813.34642	813.34644	0.02	814.35371	C28 H52 N11 O17	98.6
C30 H54 F3 N5 O17		813.3464	813.34668	0.34	814.35371	C30 H55 F3 N5 O17	98.32
C27 H46 F3 N15 O11		813.34644	813.34533	-1.36	814.35371	C27 H47 F3 N15 O11	98.17
C33 H53 F2 N5 O16		813.3464	813.34554	-1.06	814.35371	C33 H54 F2 N5 O16	98.1
C29 H47 N15 O13		813.34644	813.34778	1.65	814.35371	C29 H48 N15 O13	97.83
C24 H47 F4 N15 O12		813.34644	813.34647	0.04	814.35371	C24 H48 F4 N15 O12	97.34
C31 H50 F3 N9 O13		813.34642	813.34802	1.97	814.35371	C31 H51 F3 N9 O13	97.02
C37 H48 F N9 O11	TRUE	813.34641	813.34573	-0.84	814.35371	C37 H49 F N9 O11	96.57
C32 H48 F5 N9 O10		813.34642	813.34443	-2.44	814.35371	C32 H49 F5 N9 O10	95.97