Supporting Information - Unveiling the intricacy of gapmer oligonucleotides through advanced tandem mass spectrometry approaches and scan accumulation for 2DMS

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The Supporting information encompasses Supporting experimental mass spectra and modelled spectra, complete with detailed interpretations and mass tables. Additionally, it provides extra experimental details and the Python code for simulation, facilitating future researchers in reproducing these results.

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were included to highlight the effect of denoising)
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Section 1: Supporting Experimental Section

The denoising algorithm of sane (rank = 10) was used, which is a memory efficient development of the proposed uncoiled random QR denoising (urQRd) algorithm,¹ and is publicly available from SPIKE.² To extract the signal from the noise, the original dataset is truncated by randomly sampling the original matrix, breaking up any patterns that could contribute to the noise. This truncated dataset is then subjected to QR decomposition using a specified rank, allowing for the separation of signal and noise. After QR decomposition is applied, the resulting orthogonal matrix (Q) is multiplied by the truncated data set to reconstruct the original data with the noise removed.¹ Subsequently, QR decomposition is iterated to successive rows (t_1 rows or scan lines) until the entire matrix is factorised; this iterative approach allows for parallel processing of rows. Furthermore, the rank used in QR, which is the number of linearly independent rows/columns in the matrix used for the reconstruction of the original dataset, was previously shown to affect the quality of denoising by Chiron et al., where an optimised signal-to-noise ratio (SNR) gain was observed by selecting a rank (rank is doubled for urQRd) equivalent to the number of expected precursor ions observed in the y-axis.¹ Due to the number of precursor ions observed in Section 3.5, a logical rank of 10 was used for the denoising of danvatirsen.

Section 2: Supporting Figures



Supporting Figure S1 Nomenclature for Oligonucleotide fragmentation based on Mcluckey cleavages based on Scheme 1, where the locked nucleic acid forms a bridge between the 2 carbon and 4 carbon.



Supporting Figure S2 2D Pulse sequence, where the increment delay was fixed by the number of scans and subsequently averaged after accumulation.







Supporting Figure S4 MS spectrum of MALAT-1 after desalting HyperSep™ C18 plates.



Supporting Figure S5 MS spectrum of danvatirsen after desalting HyperSep[™] C18 plates highlighting the [M-8H]⁸⁻ and a phosphate impurity in the phosphorothioate backbone, with the simulated spectrum (bottom).



Supporting Figure S6 MS spectrum of MALAT-1 after desalting HyperSep[™] C18 plates highlighting the [M-8H]⁸⁻, a phosphate impurity in the phosphorothioate backbone, sodium and disodium adducts, with the simulated spectrum (bottom).



Supporting Figure S7 MS spectrum of danvatirsen, [M-8H]⁸⁻, with the simulated spectrum (red).



Supporting Figure S8 MS spectrum of MALAT-1, [M-8H]⁸⁻, with the simulated spectrum (red).



Supporting Figure S9 EDD-MS/MS spectrum of danvatirsen, [M-8H]⁸⁻, at 22.8 eV bias for 0.5 s irradiation time, with cleavage diagrams overlayed on top.



Supporting Figure S11 UVPD-MS/MS spectrum of danvatirsen, [M-8H]⁸⁻, using 2 shots of 3.4 mJ laser power, with cleavage diagrams overlayed on top.



Supporting Figure S12 IRMPD-MS/MS spectrum of danvatirsen, [M-8H]⁸⁻, at 27.5 % laser power for 0.06 s irradiation time, with cleavage diagrams overlayed on top.



Supporting Figure S13 Isotope pattern of w_4^{2-} ion (C₄₃H₅₄N₁₆O₂₃P₄S₄) of MALAT-1, obtained from UVPD-MS/MS (Supporting Table S4), where the peak areas (%) are overlaid on top. The A+2 peak corresponds to a molecule with one ³⁴S atom (shaded) and two ¹³C atoms, and its fine isotopic pattern allows for the resolution of these isotopes. This observation confirms the presence of four sulfur atoms, as expected for a phosphorothioate backbone.



Supporting Figure S14 Beeswarm plot of the relative intensities for each McLuckey cleavage and its analogues of MALAT-1 (Navy) and danvatirsen (Orange) produced by Tandem MS using CID, EDD, IRMPD, and UVPD. Each point represents a single peak, which is evenly spaced in the *x*-axis to prevent overlap, where 20-50% of the peaks are plotted due to the large number of peaks. Zoom-in on EDD is provided due to low abundance of peaks. Total number of peaks is overlayed on top, see Table 1.



Supporting Figure S15 The presence of an additional oxygen in danvatirsen indicates the occurrence of oxidative degradation. The observed low intensity suggests that the precursor is inherently unstable and undergoes degradation upon exposure to oxygen.



Supporting Figure S16 2D-EDD-MS of danvatirsen performed with 22.8 eV bias for 0.5 s irradiation time (1M x-axis by 2048 y-axis data points)

Supporting Figure S16A Autocorrelation line (equivalent to 1DMS, mass list available in Supporting Table S9)



Supporting Figure S16B 2DEDD-MS Fragment line extracted from the [M-6H]⁶⁻ precursor in Figure 4



Supporting Figure S16C 2DEDD-MS Fragment line extracted from the [M-7H]⁷⁻ precursor in Figure 4





Supporting Figure S16E 2DEDD-MS vertical line, which corresponds to a W_8^{3-} fragment from the autocorrelation line at m/z 922.426746, marked by an asterisk (*).



Supporting Figure S17 Fragmentation efficiency of $[M-8H]^{8-}$ danvatirsen vs. amplitude of the initial evolution pulse (Supporting Figure S2) with a 1 µs pulse length when using A) laser-based dissociation (from IR laser) and B) electron-based dissociation (from a hallow-cathode lamp operating at 22.8 eV)



Supporting Figure S18A Extracted 2DUVPD-MS/MS fragments of [M-7H]⁷⁻ precursor with denoising sane rank 10 of a single scan (top, ~350 peaks) and 8 scan accumulated (bottom, ~520 peaks).



Supporting Figure S18B Cleavage diagram of the 2DUVPD-MS/MS fragments of [M-7H]⁷⁻ after a single scan with denoising.



Supporting Figure S18C Cleavage diagram of the 2DUVPD-MS/MS fragments of [M-7H]⁷⁻ after 8 scan accumulated with denoising.



Supporting Figure S19A Extracted 2DUVPD-MS/MS fragments of [M-7H]⁷⁻ precursor without denoising of a single scan (top, ~460 peaks) and 8 scan accumulated (bottom, ~700 peaks).



Supporting Figure S19B Cleavage diagram of the 2DUVPD-MS/MS fragments of [M-7H]⁷⁻ after a single scan with denoising.



Supporting Figure S19C Cleavage diagram of the 2DUVPD-MS/MS fragments of [M-7H]⁷⁻ after 8 scan accumulated with denoising.

Section 2: Simulation of 2DMS

Expansion of Section 3.6 in the main text. Figures first show the x- and y- dimension of a 2DMS plot.



Supporting Figure S20 An ideal transient would have a steady decay in the A) x-dimension, typical of a 1DMS. Transient in B) y-dimension would remain constant assuming the spray is consistent and there is no electrostatic buildup occurring within the source or ion optics.



Supporting Figure S21 Transient in A) x-dimension and B) y-dimension with added noise ($\sim 20\%$), ideally there would be little to no noise.



Supporting Figure S22 Transient in A) x-dimension and B) y-dimension with 8-fold increase in noise compared to Supporting Figure S22, emulating the spectra of low intensity peaks.



Supporting Figure S23 A) Sum of transients generated from 2DMS (using noise threshold defined in Supporting Figure S23) and the B) Contour plot after 2DFFT, subsequent C) summation of Fourier Transformed spectra with the respective S/N calculation. Signal was determined by the maximum signal and noise adjacent to the peak was averaged.







Supporting Figure S25 Equivalent spectra as S24 but with four times the number of rows (N = 128)



Supporting Figure S26 Equivalent spectra as S24 but with eight times the number of rows (N = 256)

By comparing the signal-to-noise ratio (SNR) between Supporting Figures S24 to S26, it demonstrates that acquiring more scan limes (t_1 row) can improve the SNR. However, beyond a certain threshold, the SNR will reach a plateau where further increases in the number of scans will only result in the acquisition of more noise, which is observed in Supporting Figure S26. We therefore propose that taking multiple scans at the peak of SNR, and taking the average will lead to the greatest signal enhancement instead of acquiring more scan lines (t_1 row). Python code for simulating 2DMS is shown in page S32.



Supporting Figure S27 Zoom region of 8 scan accumulated 2DMS of danvatirsen, the presence of two distinct precursors is evident, as indicated by the presence of two intense contours—one corresponding to the [M-7H]⁷⁻ precursor and the other to a PO impurity.

Python code for simulation:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import sys
lowmass = 147
highmass = 1000
fidres = 8192 # 20=1m, 22=4m, 23=8m
noise level = 0.2
lowmassy = 300
fidresy = 256
def mz to f(data, num charge = 1):
    # data is freq or mass
    q = 1.60217662e-19 * num_charge
    B = 12 \# 12T magnet
    mol = 6.0221409e+23 *1000 #account for kg
    mz fs = (q * B * mol) / (2 * np.pi * data)
    return mz fs
def calculate frequency domain(nyq, number data points):
    #nyq rate freq * data points
    qntpoints = np.arange(0, (number_data_points))
    factor_distancy = (nyq) / (number_data_points)
    frequency domain = qntpoints * factor distancy
    return frequency domain
nyq rate = mz to f(lowmass) # get nyq rate
samp rate = 2*nyq rate # sampling rate is 2* nyq rate
transient length =fidres/samp rate #num data points / sampling rate =
transient length
nyq ratey = mz to f(lowmassy) # get nyq rate
samp ratey = 2*nyq ratey # sampling rate is 2* nyq rate
transient lengthy = fidresy/samp ratey
sample freq 622 = mz to f(622) #select a mass e.g. 622 and convert to
frequency
print(nyq rate: %.2f\nfid len: %.2f\nsample freq: %.2f%(nyq rate,
transient length, sample freq 622))
tx = np.linspace(0, transient length, fidres) #x dimension
ty = np.linspace(0,transient lengthy,fidresy) #y dimension
X, Y = np.meshgrid(tx, ty) #create 2D array of x and y data points
xdim = np.exp(1j * sample freq 622 * np.pi * X) * np.exp(sample freq 622*-X
* 0.002) # xdim and damping transient
ydim = np.exp(1j * sample freq 622 * np.pi * Y) #ydim with no damping added
f = xdim*ydim
#Add noise in x and y dimension
f noise = f + (np.random.normal(0,noise level,size=np.shape(f))) #+ (1j *
np.random.normal(0,noise level,size=np.shape(f)))
ft = np.fft.rfft2(f) # 2d fft take real spectrum
ft = np.fft.fftshift(ft) #reorder the fft data set so peaks are centered
fig, axes = plt.subplots(3, figsize=(6,8))
```

```
axes[0].plot(np.sum(f_noise,axis=0),c=k) #Sum all the rows and plot the FID
# Annotate the plot
axes[0].plot([],[], , label=Sum of %s $t_{1}$ rows%fidresy)
axes[0].set_title(A, loc=left)
axes[0].set_ylabel(Intensity)
axes[0].legend(frameon=False,loc=best, bbox_to_anchor=(0.2, 0.5, 0.8, 0.8))
```

```
data_points_x = len(ft[0])
ft = np.sqrt((np.power(ft.real, 2)) + (np.power(ft.imag, 2)))
```

```
#Plot 2D contour plot
axes[1].contour(ft,cmap=gray,levels=4)
axes[1].set_yticks(np.arange(0, 10+1, 2))
axes[1].set_ylim([int(fidresy)/1.8,int(fidresy)/1.5])
axes[1].set_xlim([2528,2535]) #select range to see peak
axes[1].set_title(B, loc=left)
axes[1].set_ylabel(Index / y)
```

```
ft1d = np.sum(ft[:, :], axis=0) #Sum all FTs
sig = np.max(ft1d) # select the max signal
noise = np.mean(ft1d[2000:2400]) # mean noise (magnitude mode) of noise
adjacent to signal
```

```
SN = sig/noise
print(Sig = %.2f \nNoise = %.2f\nSN=%.2f%(sig,noise,sig/noise))
```

```
# Plot the summated FTs
axes[2].plot(ft<sub>1</sub>d,c=k)
axes[2].plot([],[], , label=S/N = %.2f%(SN))
axes[2].set_xlim([2500,2560]) #adjust range to see peak
axes[2].legend(frameon=False)
axes[2].set_title(C, loc=left)
axes[2].set_ylabel(Intensity)
```

```
plt.show()
```

Section 3: Code for generating oligonucleotide mass list.

Available at https://github.com/MKRahman97/Oligonucleotide_mass_calculator.



Supporting Figure S27 Define the inputs for the oligonucleotide mass calculator by customising the elemental formula for the coloured regions.

Section 4: Tables of peak lists

Table S1 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ MALAT-1 by EDD MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured	S/N	Elemental	Theoretical	Error	Charge	Assignment	
mz		Composition	mz	(ppm)			
165.949499 317.024092	27.7 33.6	$C_{10}H_{13}N_3O_5PS$	317.024077	- 0.048	-1	w11(mC)b6 - H2O, w4(mC)b13 -	J1
319.015912	26.6	$C_{10}H_{13}N_2O_6PS$	319.015918	0.019	-1	H2O, x1 - OCH2 x10(T)b7, y10(T)c7, z10(T)d7, b5(T)x12	J2
						x7(T)b10, c5(T)y12, a7(T)w10, z7(T)d10, d5(T)z12,	
						a5(T)w12, b7(T)x10, c7(T)y10, d7(T)z10, a10(T)w7, b10(T)x7	
						c10(T)y7, d10(T)z7, y7(T)c10, d4(T)z13, w7(T)a10,	
						z13(T)d4, x12(T)b5, c4(T)y13, y12(T)c5, w12(T)a5,	
						w13(T)a4, y13(T)c4, b4(T)x13, x13(T)b4, z12(T)d5, w10(T)a7	
327.019667	35.9	$C_{10}H_{11}N_5O_4PS$	327.019661	-	-1	w10(1)a7, a4(T)w13 w8(A)b9 - H2O, x5a12, w9(A)b8	J3
				0.019		- H2O, w6(A)b11 - H2O	
328.027493	19.0	$C_{10}H_{12}N_5O_4PS$	328.027486	- 0.021	-1	x5a12 + 1H, a8(A)w9, w9(A)a8, x9(A)b8, v9(A)b8,	J4
						z9(A)d8, w8(A)a9, y8(A)c9, z8(A)d9,	
						w6(A)a11, x6(A)b11, y6(A)c11, z6(A)d11, b8(A)v0	
						c12(G)z5, c8(A)y9, z5(G)c12, d8(A)z9.	
						a9(A)w8, b9(A)x8, c9(A)v8.	

d9(À)z8. c11(Å)y6, a12(G)x5, d11(A)z6 332.406213 15.8 332.468783 34.4 356.904022 356.8 416.841796 23.1 418.904416 64.2 470.054137 C₁₆H₁₈N₅O₈PS 470.054094 z2 - B(dC) -16.8 -1 -OCH2 0.092 521.043300 11.0 $C_{63}H_{78}N_{26}O_{32}P_6S_6$ 521.043359 0.114 -4 w6 546.038427 16.4 d5 577.374574 18.6 $C_{53}H_{66}N_{17}O_{30}P_5S_5$ 577.374495 -3 0.138 w5 585.381470 C53H66N21O28P5S5 585.381984 -3 15.1 0.879 w7 601.048682 25.7 C₇₃H₉₁N₂₈O₃₈P₇S₇ 601.049158 0.791 -4 631.422997 11.1 b6 - H2O, a6 -645.736608 26.0 C₆₃H₇₇N₂₀O₃₂P₅S₅ 645.736204 -3 2H 0.625 647.929731 33.2 $C_{166}H_{214}N_{60}O_{84}P_{15}S_{15}$ 647.934574 7.475 -8 M - 8H2O 654.923646 10.5 656.948065 11.8 661.064312 12.5 M - 8H 11192.9 -8 664.810898 C₁₆₆H₂₀₅N₆₀O₈₄P₁₅S₁₅ 664.811336 0.659 w10 676.256998 $C_{103}H_{128}N_{40}O_{52}P_{10}S_{10}$ 676.256415 24.0 -5 0.862 w8 683.307803 27.8 C₈₃H₁₀₃N₃₃O₄₂P₈S₈ 683.307848 0.066 -4 b9 - B(dG) - 2H, 694.809922 $C_{88}H_{109}N_{27}O_{46}P_8S_8$ 694.809890 24.6 -4 b9 - B(A) - H2O 0.046 w4 706.061335 52.9 $C_{43}H_{54}N_{16}O_{23}P_4S_4$ 706.061776 0.624 -2 712.468903 19.7 $C_{113}H_{139}N_{39}O_{56}P_{10}S_{10}$ 712.468947 0.062 b11 - H2O, a11 -5 - 2H M - 7H - NH3 --7 721.483760 14.5 $C_{156}H_{190}N_{55}O_{80}P_{15}S_{15}$ 721.483651 2T 0.151 728.573657 27.7 C₉₃H₁₁₄N₃₂O₄₆P₈S₈ 728.573513 -4 b9 - H2O, a9 -2H 0.198 737.061618 18.3 $C_{22}H_{28}N_8O_{13}P_2S_2$ 737.061973 0.482 w2, d2 -1 740.492242 259.4 M - 7H - 4H - $C_{161}H_{199}N_{55}O_{84}P_{15}S_{15}$ 740.490806 -7 dA 1.939 a7 - 2H, b7 -752.411054 34.9 $C_{73}H_{90}N_{22}O_{38}P_6S_6$ 752.410602 -3 H2O 0.600 M - 7H - 4H 759.784631 150.7 $C_{166}H_{204}N_{60}O_{84}P_{15}S_{15}$ -7 759.784305 0.429 z7 - 2H, y7 -763.750269 24.6 C₇₃H₈₈N₂₈O₃₅P₆S₆ 763.749952 -3 H2O 0.415 w9 765.566883 765.566539 5.2 $C_{93}H_{115}N_{38}O_{46}P_9S_9$ -4 0.449 778.479254 10.3 z12 - 2H, y12 -781.274275 62.2 $C_{123}H_{152}N_{45}O_{60}P_{11}S_{11}$ 781.278079 -5 4.869 H2O 801.733790 7.4 C₇₃H₉₁N₂₈O₃₈P₇S₇ 801.734636 1.055 -3 w7 804.068697 804.068889 w12 7.8 $C_{123}H_{155}N_{45}O_{63}P_{12}S_{12}$ 0.239 -5 809.076385 23.7 y10 - H2O, z10 817.083648 30.1 $C_{103}H_{125}N_{40}O_{49}P_9S_9$ 817.083825 0.216 -4 - 2H y5 - H2O, z5 -821.600305 8.7 C₅₃H₆₃N₂₁O₂₅P₄S₄ 821.599588 _ -2 2H 0.873 830.604948 14.2 $C_{53}H_{65}N_{21}O_{26}P_4S_4$ 830.604871 -2 y5 0.092

x8(A)b9, a11(A)w6, b11(A)x6,

842.733073 845.282848	10.0 14.2	$C_{133}H_{165}N_{47}O_{66}P_{12}S_{12}$	845.282718	- 0.154	-5	z13 - 2H, y13 - H2O, a13 - 2H, b13 - H2O
861.752810	13.6					
863.906735	7.5	$C_{161}H_{198}N_{55}O_{84}P_{15}S_{15}$	863.905849	- 1 025	-6	M - 8H - dA
873.427857	15.8	$C_{83}H_{100}N_{33}O_{39}P_7S_7$	873.428206	0.400	-3	z8 - 2H, y8 - H2O
878.575916	11.4	$C_{53}H_{66}N_{21}O_{28}P_5S_5$	878.576614	0.795	-2	w5
886.414777	24.6	$C_{166}H_{203}N_{60}O_{84}P_{15}S_{15}$	886.414931	0.174	-6	M - 8H
896.843821	5.5	$C_{113}H_{139}N_{43}O_{54}P_{10}S_{10}$	896.843619	- 0.225	-4	y11 - H2O, z11 - 2H
911.414020	8.6	$C_{83}H_{103}N_{33}O_{42}P_8S_8$	911.412890	-	-3	w8
				1.240		
925.582584	13.4	$C_{113}H_{143}N_{43}O_{57}P_{11}S_{11}$	925.584089	1.626	-4	w11 + 1H
926.747840	23.1	$C_{88}H_{109}N_{27}O_{46}P_8S_8$	926.748945	1.193	-3	b9 - B(A) - H2O, b9 - B(dG) - 2H
968.603923	28.3					· · ·
971.430996	26.1					
976.843282	10.1					
983.105775	15.1	$C_{93}H_{112}N_{38}O_{43}P_8S_8$	983.106460	0.696	-3	z9 - 2H, y9 - H2O
1021.425317	12.6	$C_{93}H_{116}N_{38}O_{46}P_9S_9$	1021.427086	1.732	-3	w9 + 1H
1043.094482	6.9	$C_{63}H_{78}N_{26}O_{32}P_6S_6$	1043.093995	-	-2	w6
				0.467		
1094.091304	12.2	$C_{33}H_{40}N_{13}O_{18}P_3S_3$	1094.091650	0.317	-1	w3, d3
1129.117194	9.9			0 740		
			Abs mean error	0.710		
			Abs mean std dev	0.898		

Table S2 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ MALAT-1 by CID MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured	S/N	Elemental	Theoretical	Error	Charg	Assignmen	
mz		Composition	mz	(ppm)	е	t	
319.015918	231.5	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	0.000	-1	x10(T)b7, y10(T)c7, z10(T)d7, b5(T)x12, x7(T)b10, c5(T)y12, a7(T)w10, z7(T)d10, d5(T)z12, a5(T)w12, b7(T)x10, c7(T)y10, d7(T)z10, a10(T)w7, b10(T)x7, c10(T)y7, d10(T)z7, y7(T)c10, d4(T)z13, w7(T)a10, z13(T)d4, x12(T)b5, c4(T)y13, y12(T)c5, w13(T)a4, y13(T)c4, b4(T)x13, x13(T)b4, z12(T)d5, w10(T)a7, a4(T)w13	J 1
328.027433	81.8	C ₁₀ H ₁₂ N ₅ O ₄ PS	328.027486	0.163	-1	x5a12 + 1H, a8(A)w9, w9(A)a8, x9(A)b8, y9(A)c8, z9(A)d8, w8(A)a9, y8(A)c9, z8(A)d9, w6(A)a11, x6(A)b11, y6(A)c11, z6(A)d11, z6(A)d11, z6(A)d11, z6(A)d11, z6(A)d11, z6(A)d2, z5(G)c12, d8(A)z9, a9(A)w8, b9(A)x8, c9(A)y8, x8(A)b9, a11(A)w6, b11(A)x6, d9(A)z8, c11(A)y6, a12(G)x5, d11(A)z6	J 2
337.026466	41.6	$C_{10}H_{15}N_2O_7PS$	337.026483	0.050	-1	y13(T)d4 + 2H, y12(T)d5 + 2H, y10(T)d7 + 2H, y7(T)d10 + 2H, b4(T)w13 + 2H.	J 3

344.022387	48.4	$C_{10}H_{12}N_5O_5PS$	344.022400	0.037	-1	w12(T)b5 + 1H, b5(T)w12 + 2H, b7(T)w10 + 2H, d7(T)y10 + 2H, d10(T)y7 + 2H, b10(T)w7 + 2H, w13(T)b4 + 1H, w13(T)b4 + 1H, w10(T)b7 + 1H, d4(T)y13 + 2H, d5(T)y12 + 2H d12(G)z5, x5(G)b12, y5(G)c12, w5(G)a12, y6(A)a8, d8(A)y9, c12(G)y5, b9(A)w8, d9(A)y8, b12(G)x5, a12(G)w5, y8(A)a9	J 4
346.026698	39.2	$C_{11}H_{14}N_3O_6PS$	346.026817	0.345	-1	yo(A)d3, b11(A)w6, d11(A)y6 z15(dC)d2, d2(dC)z15, c2(dC)y15, b2(dC)x15, a2(dC)w15, w15(dC)a2, x15(dC)b2, w1 - H2O, y15(dC)c2	J 5
352.984562 356.022292 364.025674	163.8 336.9 64.3	C ₁₁ H ₁₂ N ₅ O ₅ PS	356.022400	0.303	-1	b14(dA)x3, z3(dA)d14, d3(dA)z14, w14(dA)a3, a14(dA)w3, c14(dA)y3, y3(dA)c14, x3(dA)b14, x2a15 + 1H, c3(dA)y14, a15(dG)x2, b3(dA)x14, z2(dG)c15, a3(dA)w14, c15(dG)z2, x14(dA)c3, y14(dA)c3, z14(dA)d3, w3(dA)a14, d14(dA)z3 d3, w3	J 6
368.025674 368.027117	64.3 1926. 7	C ₃₃ H ₄₀ N ₁₃ O ₁₈ P ₃ S ₃ C ₂₂ H ₂₈ N ₈ O ₁₃ P ₂ S ₂	364.025699 368.027348	0.070 0.628	-3 -2	u3, w3 w2, d2	
368.528995 371.493430	254.0 138.2	$C_{48}H_{56}N_{15}O_{24}P_4S_4$	368.529122	0.344	-4	a5 - B(T) - H2O	
390.027761	88.7	$C_{11}H_{14}N_5O_7PS$	390.027880	0.305	-1	d15(dG)y2 + 2H, w2b15 + 1H, y2d15 + 2H, b15(dG)w2 + 2H, d1	J 7
414.959406	131.5	$C_{10}H_{14}N_2O_8P_2S_2$	414.959405	- 0.001	-1	x12(T)d5 + 1H, x13(T)d4 + 1H, d10(T)x7, c10(T)w7, c7(T)w10,	J 8

d7(T)x10, x10(T)d7 + 1H, d5(T)x12, c5(T)w12, x7(T)d10 + 1H, w13(T)c4, w12(T)c5, d4(T)x13, w10(T)c7, c4(T)w13, w7(T)c10

417.052764 420.511784 421.01350 426.064272	4 114.1 4 605.3 7 99.0 2 43.2					
438.78492	1 62.2	$C_{53}H_{66}N_{21}O_{28}P_5S_5$	438.784669	- 0.573	-4	w5
453.626744 470.054300	4 13.5 0 11.4	C ₆₈ H ₈₆ N ₂₃ O ₃₈ P ₇ S ₇ C ₁₆ H ₁₈ N ₅ O ₈ PS	453.626972 470.054094	0.503 - 0.439	-5 -1	w7 - B(dA) z2 - B(dC) - OCH2
479.008380 480.638072	2 70.5	$C_{73}H_{91}N_{28}O_{38}P_7S_7$	480.637871	- 0.417	-5	w7
487.280148	3 19.9	$C_{58}H_{73}N_{21}O_{32}P_6S_6$	487.279736	- 0.847	-4	w6 - B(dA)
494.985659 498.570129 503.997019	9 99.6 5 140.2 5 56.8	$C_{33}H_{39}N_{13}O_{16}P_2S_2$	498.570443	0.638	-2	b3, y3
512.53918	7 28.9 3 283 0	$C_{63}H_{80}N_{20}O_{35}P_6S_6$	512.538847	- 0.663	-4	d6
519.434148	3 200.0 3 25.1	$C_{78}H_{98}N_{28}O_{42}P_8S_8$	519.433924	- 0.431	-5	w8 - B(A)
521.04295	9 74.7	$C_{63}H_{78}N_{26}O_{32}P_6S_6$	521.043359 535.032181	0.767	-4	w6 x5 - B(dA) +
537 53654	7 12 1	CasHaaNaaOa-PaSa	537 53600/	0.214	-0	1H, w5 - B(dG) w3 - H2O d3 -
	1 12.1		557.550304	0.000	-2	H2O
545.39319	3 73.2	C ₅₃ H ₆₅ N ₁₇ O ₂₈ P ₄ S ₄	545.393333	0.257	-3	b5
546.542130	55.3	$C_{33}H_{40}N_{13}O_{18}P_3S_3$	546.542187	0.104	-2	w3, d3
553.400379 558.431030 563.291658	9 270.0 0 27.5 3 22.3	$C_{53}H_{65}N_{21}O_{26}P_4S_4$	553.400822	0.801	-3	y5
567.28465	5 1117. 4	$C_{68}H_{86}N_{23}O_{38}P_7S_7$	567.285534	1.550	-4	w7 - B(dA)
577.06347	5 7.3	$C_{73}H_{90}N_{28}O_{36}P_6S_6$	577.063286	- 0.328	-4	у7
579.378084	4 15.4	$C_{53}H_{64}N_{21}O_{27}P_5S_5$	579.378462	0.653	-3	w5 - H2O
585.381229	9 743.9	$C_{53}H_{66}N_{21}O_{28}P_5S_5$	585.381984	1.289	-3	w5
594.044080) 10.2	$C_{108}H_{137}N_{38}O_{57}P_{11}S_1$	594.043247	-	-6	w11 - B(A)
604 04000	0 6470			1.402	4	w7
601.04836	5 647.3	$C_{73}H_{91}N_{28}O_{38}P_7S_7$	601.049158	1.323	-4	W_{i}
604.050724	+ 23.8	C ₅₈ H ₇₀ N ₁₇ O ₃₁ P ₅ S ₅	604.049900	- 1.364	-3	H2O, b6 - B(T) - NH3
612.551382	2 25.2	$C_{78}H_{97}N_{22}O_{42}P_7S_7$	612.551199	- 0.298	-4	b8 - B(A) - H2O, b8 - B(dG) - 2H
616.552784	4 5.3	C ₁₁₃ H ₁₄₂ N ₄₃ O ₅₇ P ₁₁ S ₁	616.552329	- 0.738	-6	w11
618.060884	4 14.2	$C_{58}H_{72}N_{21}O_{30}P_5S_5$	618.060910	0.042	-3	y6 - B(dA)
623.25411	5 5.7	$C_{98}H_{124}N_{29}O_{53}P_9S_9$	623.253208	-	-5	b10 - B(A)
				1.456		

625.558645	12.3	$C_{78}H_{97}N_{28}O_{40}P_7S_7$	625.558353	-	-4	y8 - B(A)
631.046723	862.7	$C_{155}H_{189}N_{57}O_{79}P_{15}S_1$	631.047711	0.467 1.565	-8	c15 - 2H
631.547134	16.0	$\overset{\circ}{C}_{38}H_{51}N_{11}O_{22}P_4S_4$	631.544896	- 3.544	-2	w4 - B(dG) + 2H
641.117889 646.934278	137.6 20.8	$C_{22}H_{27}N_8O_{11}PS$	641.118485	0.930	-1	b2, y2
647.929370	923.4	$C_{166}H_{214}N_{60}O_{84}P_{15}S_1$	647.934574	8.030		M - 8H2O
649.544672	29.5	$C_{78}H_{98}N_{28}O_{42}P_8S_8$	649.544225	- 0.688	-4	w8 - B(A)
658.085694 658.090197	74.2 143.5	$C_{43}H_{53}N_{16}O_{21}P_3S_3$	658.090032	-	-2	у4
659.322365	27.1	$C_{83}H_{102}N_{33}O_{40}P_7S_7$	659.321977	0.251 - 0.589	-4	у8
663.079559	39.3	$C_{63}H_{77}N_{26}O_{30}P_5S_5$	663.079076	- 0.729	-3	у6
663.748775	8.0	$C_{63}H_{79}N_{26}O_{30}P_5S_5$	663.750959	3.291	-3	y6 + 2H
664.809983	1777. 2	$\begin{array}{c} C_{166}H_{205}N_{60}O_{84}P_{15}S_{1}\\ {}_{5}\end{array}$	664.811336	2.036	-8	M - 8H
665.850084	46.5	C ₁₀₃ H ₁₂₈ N ₃₄ O ₅₄ P ₁₀ S ₁ 0	665.850692	0.912	-5	d10 - H2O
670.050543	8.6	$C_{83}H_{102}N_{27}O_{44}P_8S_8$	670.048739	- 2.692	-4	c8 - 2H
670.301131	47.1	$C_{83}H_{103}N_{27}O_{44}P_8S_8$	670.300695	- 0.651	-4	d8 - H2O
677.717028	14.8	$C_{63}H_{78}N_{20}O_{34}P_6S_6$	677.717366	0.499	-3	d6 - H2O
678.805739	8.6	$C_{83}H_{101}N_{33}O_{41}P_8S_8$	678.805207	- 0 784	-4	W8 - H2O
683.807106	20.3			0.704		
683.809895	33.2		005 4500 40		-	
685.458357	154.9	C ₁₀₈ H ₁₃₄ N ₃₄ O ₅₆ P ₁₀ S ₁ 0	685.458048	- 0.450	-5	2H, b11 - B(A) - H2O
689.057419	14.9	$C_{63}H_{76}N_{26}O_{31}P_6S_6$	689.056716	- 1.021	-3	w6 - H2O
694.809383	1615. 6	$C_{88}H_{109}N_{27}O_{46}P_8S_8$	694.809890	0.729	-4	b9 - B(dG) - 2H, b9 - B(A) - H2O
697.056953	32.6	$C_{43}H_{52}N_{16}O_{22}P_4S_4$	697.056494	- 0.658	-2	w4 - H2O
697.549218	18.1	$C_{43}H_{51}N_{15}O_{23}P_4S_4$	697.548501	- 1.028	-2	w4 - NH3, d4 - H2O
703.476698	8.4	$C_{151}H_{184}N_{53}O_{78}P_{15}S_1$	703.477519	1.167	-7	M - 7H - NH3 - 3T
706.061808	88.1	$C_{43}H_{54}N_{16}O_{23}P_4S_4$	706.061776	- 0.045	-2	w4
713.054218	5.2	C ₁₀₈ H ₁₃₇ N ₃₈ O ₅₇ P ₁₁ S ₁	713.053351	- 1.216	-5	w11 - B(A)
716.071767	5.4	$C_{113}H_{141}N_{39}O_{57}P_{10}S_1$	716.071060	- 0.988	-5	b11
720.225655	9.0	C ₁₃₃ H ₁₆₆ N ₄₇ O ₆₈ P ₁₃ S ₁ 3	720.224967	- 0.955	-6	w13 - H2O, d13 - H2O
721.341468	476.6	$\begin{array}{c} C_{155}H_{189}N_{57}O_{79}P_{15}S_{1}\\ {}_{5}\end{array}$	721.341281	- 0.260	-7	c15 - 2H
724.736138	47.2	$C_{68}H_{85}N_{23}O_{36}P_6S_6$	724.735309	- 1.144	-3	y7 - B(dA)
728.068317	18.7	$C_{68}H_{83}N_{25}O_{35}P_6S_6$	728.067170	- 1.575	-3	y7 - B(mC)

736.091701	22.5					
738.494095	23.5		744 020240		e	614 - B(A) -
741.230883	11.6	G ₁₃₉ H ₁₇₂ N ₄₇ O ₇₁ P ₁₃ S ₁ 3	741.230249	- 0.856	-0	H2O, b14 - B(G) - 2H
747.091318	70.6					
751.265622	5.8	C ₁₁₈ H ₁₄₆ N ₃₉ O ₆₀ P ₁₁ S ₁ 1	751.265000	- 0.827	-5	b12 - B(G) - H2O, z12 - B(A) - NH3
752.411492	50.9	$C_{73}H_{90}N_{22}O_{38}P_6S_6$	752.410602	- 1 183	-3	a7 - 2H, b7 - H2O
755 079986	18.4		755 080166	0.239	-2	z5 - B(dA)
756.716866	14.6	$C_{68}H_{86}N_{23}O_{38}P_7S_7$	756.716471	- 0 522	-3	w7 - B(dA)
763.740349	19.5	$C_{144}H_{177}N_{52}O_{71}P_{13}S_1$	763.739332	-	-6	b14 - H2O, y14 - H2O, z14 -
700 077000	0.0	, о н м о ро	700 075445		0	2H, a14 - 2H
768.077326	9.8	$C_{48}H_{58}N_{18}O_{25}P_4S_4$	768.075415	- 2.489	-2	у5 - B(dC)
769.753799	374.0	$C_{73}H_{90}N_{28}O_{36}P_6S_6$	769.753474	- 0.422	-3	y/
774.816636	7.5	$C_{98}H_{122}N_{29}O_{52}P_9S_9$	774.815688	- 1.223	-4	b10 - B(dG) - 2H, b10 - B(A) -
784.392792	8.0	C ₇₃ H ₉₁ N ₂₂ O ₄₀ P ₇ S ₇	784.391765	-	-3	H2O d7 - H2O
				1.309		
801.734165	9.8	$C_{73}H_{91}N_{28}O_{38}P_7S_7$	801.734636	0.587	-3	w7
808.579758	35.9	$C_{103}H_{127}N_{34}O_{52}P_9S_9$	808.579312	-	-4	a10 - 2H, b10 -
				0.552		H2O
809.587847	59.1	$C_{53}H_{63}N_{17}O_{27}P_4S_4$	809.588355	0.627	-2	b5 - H2O, a5 - 2H
815.009010	22.5					
817.070655	396.8	$C_{78}H_{97}N_{22}O_{42}P_7S_7$	817.070691	0.044	-3	b8 - B(dG) - 2H, b8 - B(A) - H2O
818.594763	21.6	$C_{53}H_{65}N_{17}O_{28}P_4S_4$	818.593637	- 1 376	-2	b5
823.811700	281.0			1.570		
824.020052	29.3					
830.603910	1217. 8	$C_{53}H_{65}N_{21}O_{26}P_4S_4$	830.604871	1.157	-2	y5
841.733835	6.4	$C_{156}H_{191}N_{56}O_{79}P_{15}S_1$	841.734803	1.150	-6	M - 6H - H2O - 2T
857.074832	80.4	$\tilde{C}_{108}H_{134}N_{34}O_{56}P_{10}S_1$	857.074379	- 0 528	-4	b11 - B(A) - H2O, b11 -
862.089961	12.0	° C ₈₃ H₁02N27O₄2P7S7	862.088856	-	-3	B(dG) - 2H b8 - H2O, a8 -
070 570075	10 5		070 5700//	1.282		2H
878.578075	42.5	$C_{53}H_{66}N_{21}O_{28}P_5S_5$	878.576614	- 1.663	-2	W5
885.063632	34.8					
906.577844	312.0	$C_{58}H_{70}N_{17}O_{31}P_5S_5$	906.578488	0.710	-2	b6 - B(mC) - H2O, b6 - B(T)
907.582273	24.4	$C_{57}H_{70}N_{18}O_{31}P_5S_5$	907.580025	- 2 477	-2	- NH3 b6 - B(T) - CH3
926.748741	265.9	$C_{88}H_{109}N_{27}O_{46}P_8S_8$	926.748945	0.220	-3	b9 - B(A) - H2O, b9 -
040450404	40.0					B(dG) - 2H
942.158461	18.0		000 407044		0	
969.109520	12.6	$C_{63}H_{77}N_{20}O_{32}P_5S_5$	969.107944	- 1.627	-2	ao - 2n, no - H2O
980.138069	18.9	$C_{33}H_{37}N_{13}O_{15}P_2S_2$	980.137597	- 0 481	-1	y3 - H2O, a3 - 2H, b3 - H2O,
000 440 400			000 440400	0.701	4	z3 - 2H
998.148489	154.5	$ $	998.148162	-	-1	us, ys

				0.328		
999.153265	35.9					
1094.09195	11.8	C ₃₃ H ₄₀ N ₁₃ O ₁₈ P ₃ S ₃	1094.09165	-	-1	w3, d3
5			0	0.278		
1226.11099	8.8	C ₇₈ H ₉₇ N ₂₂ O ₄₂ P ₇ S ₇	1226.10967	-	-2	b8 - B(dG) - 2H_b8 - B(A) -
4			5	1.075		H2O
			Abs mean	0.856		
			error			
			Abs mean	0.609		
			std dev			
Table S3 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ MALAT-1 by IRMPD MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured <i>mz</i>	S/N	Elemental Composition	Theoretical <i>mz</i>	Error (ppm)	Charg e	Assignmen t	
150.042285 192.973096 193.976452 194.968900 211.165591 255.994508	32.6 974.9 49.3 38.5 50.0 233.5			,			
319.015934	130.4	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	0.050	-1	x10(T)b7, y10(T)c7, z10(T)d7, b5(T)x12, x7(T)b10, c5(T)y12, a7(T)w10, z7(T)d10, d5(T)z12, a5(T)w12, b7(T)x10, c7(T)y10, d7(T)z10, a10(T)w7, b10(T)x7, c10(T)y7, d10(T)z7, y7(T)c10, d4(T)z13, w7(T)a10, z13(T)d4, x12(T)b5, c4(T)y13, y12(T)c5, w13(T)a4, y13(T)c4, b4(T)x13, x13(T)b4, z12(T)d5, w10(T)a7, w10(T)	J 1
328.027483	55.5	C ₁₀ H ₁₂ N ₅ O ₄ PS	328.027486	0.008	-1	x5a12 + 1H, a8(A)w9, w9(A)a8, x9(A)b8, y9(A)c8, z9(A)d8, w8(A)a9, y8(A)c9, z8(A)d9, w6(A)a11, x6(A)b11, y6(A)c11, z6(A)d11, b8(A)x9, c12(G)z5, c8(A)y9, z5(G)c12, d8(A)z9, a9(A)w8, b9(A)x8, c9(A)y8, x8(A)b9, a11(A)w6, b11(A)x6, d9(A)z8, c11(A)y6	J 2

337.026480 346.026794	63.5	$C_{10}H_{15}N_2O_7PS$ $C_{11}H_{14}N_3O_6PS$	337.026483 346.026817	0.008	-1	a12(G)x5, d11(A)z6 y13(T)d4 + 2H, y12(T)d5 + 2H, y10(T)d7 + 2H, y7(T)d10 + 2H, b4(T)w13 + 2H, w12(T)b5 + 1H, b5(T)w12 + 2H, b7(T)w10 + 2H, d7(T)y10 + 2H, d10(T)y7 + 2H, w7(T)b10 + 1H, w13(T)b4 + 1H, w10(T)b7 + 1H, d4(T)y13 + 2H, d5(T)y12 + 2H z15(dC)d2, d2(dC)z15, c2(dC)y15, b2(dC)x15, a2(dC)w15, w15(dC)a2, x15(dC)b2, w1 - H2O, y15(dC)c2	J 3 J 4
352.984577 356.022396 364.025690	147.9 67.0	CasH40N40O49PaSa	356.022400	0.011	-1	b14(dA)x3, z3(dA)d14, d3(dA)z14, w14(dA)a3, a14(dA)w3, c14(dA)y3, y3(dA)c14, x3(dA)b14, x2a15 + 1H, c3(dA)y14, a15(dG)x2, b3(dA)x14, z2(dG)c15, a3(dA)w14, c15(dG)z2, x14(dA)b3, y14(dA)c3, x14(dA)d3, w3(dA)a14, d14(dA)z3 d3, w3	J 5
368.027344 371.493471	193.6 39.7	$C_{22}H_{28}N_8O_{13}P_2S_2$	368.027348	0.010	-3 -2	w2, d2	
390.027942	26.0	$C_{11}H_{14}N_5O_7PS$	390.027880	- 0.158	-1	d15(dG)y2 + 2H, w2b15 + 1H, y2d15 + 2H, b15(dG)w2 + 2H, d1	J 6
398.982201 414.959366 417.052648	32.0 94.5 138.6	C ₁₀ H ₁₄ N ₂ O ₈ P ₂ S ₂	414.959405	0.094	-1	x12(T)d5 + 1H, x13(T)d4 + 1H, d10(T)x7, c10(T)w7, c7(T)w10, d7(T)x10, x10(T)d7 + 1H, d5(T)x12, c5(T)w12, x7(T)d10 + 1H, w13(T)c4, w12(T)c5, d4(T)x13, w10(T)c7, c4(T)w13, w7(T)c10	J 7

418.055928 420.511859	22.0 100.6						
432.969924	52.9	$C_{10}H_{16}N_2O_9P_2S_2$	432.969970	0.107	-1	d7(T)w10 + 2H, w7(T)d10 + 2H, d10(T)w7 + 2H, d5(T)w12 + 2H, w13(T)d4 + 2H, d4(T)w13 + 2H, w10(T)d7 + 2H, w12(T)d5 + 2H	J 8
442.059113 453.626957 470.054057	76.2 18.6 64.3	C ₆₈ H ₈₆ N ₂₃ O ₃₈ P ₇ S ₇ C ₁₆ H ₁₈ N ₅ O ₈ PS	453.626972 470.054094	0.033 0.080	-5 -1	w7 - B(dA) z2 - B(dC) -	
470.372095	41.4	$C_{43}H_{54}N_{16}O_{23}P_4S_4$	470.372092	- 0.006	-3	w4	
479.008402 480.637956	41.4 29.5	$C_{73}H_{91}N_{28}O_{38}P_7S_7$	480.637871	- 0.176	-5	w7	
494.985500 495.988907 498.570350 503.997091 512.996053	84.1 15.3 37.8 41.2 1684.	$C_{33}H_{39}N_{13}O_{16}P_2S_2$	498.570443	0.186	-2	b3, y3	
513.999466 515.000378 522.007646 538.002603 545.054822	0 266.3 33.9 25.7 80.7 97.0						
553.400759 554.065887	129.9 23.1	$C_{53}H_{65}N_{21}O_{26}P_4S_4$	553.400822	0.114	-3	у5	
567.285847	577.0	$C_{68}H_{86}N_{23}O_{38}P_7S_7$	567.285534	- 0.551	-4	w7 - B(dA)	
577.063399	23.4	$C_{73}H_{90}N_{28}O_{36}P_6S_6$	577.063286	- 0 195	-4	у7	
580.056287	16.7	$C_{92}H_{113}N_{32}O_{46}P_8S_8$	580.055790	- 0 857	-5	a9 - CH3	
585.382052	234.5	$C_{53}H_{66}N_{21}O_{28}P_5S_5$	585.381984	- 0 117	-3	w5	
586.047104	46.8	$\begin{array}{c} C_{127}H_{157}N_{44}O_{66}P_{12}S_{1}\\ {}_{2}\end{array}$	586.046745	- 0.612	-7	b13 - B(mC) - CH3	
597.305980 601.049588	13.9 476.6	$C_{73}H_{91}N_{28}O_{38}P_7S_7$	601.049158	- 0 716	-4	w7	
604.384341 612.551467	63.6 20.7	$C_{78}H_{97}N_{22}O_{42}P_7S_7$	604.385842 612.551199	2.484 - 0.437	-3 -4	a6 - B(mC) b8 - B(A) - H2O, b8 - B(dG) - 2H	
618.060944	23.4	$C_{58}H_{72}N_{21}O_{30}P_5S_5$	618.060910	- 0.055	-3	y6 - B(dA)	
630.922877	57.2	$C_{156}H_{194}N_{50}O_{84}P_{15}S_1$	630.921734	- 1 811	-8	M - 8H - 4H - 2dA	
631.547891	6.5	$\overset{\circ}{C}_{38}H_{51}N_{11}O_{22}P_4S_4$	631.544896	- 4 742	-2	w4 - B(dG) + 2H	
641.118365 642.121779	271.4 60.6	$C_{22}H_{27}N_8O_{11}PS$	641.118485	0.187	-1	b2, y2	
647.927175	876.3	$C_{161}H_{200}N_{55}O_{84}P_{15}S_{15}$	647.929524	3.625		M - 8H - dA	
650.818018	5.0	$C_{83}H_{104}N_{27}O_{43}P_7S_7$	650.817464	- 0.852	-4	b8	
658.089902 658.447318	87.0 29.8	$C_{43}H_{53}N_{16}O_{21}P_3S_3$	658.090032	0.198	-2	y4	

658.581878 661.046256 663.061388	38.6 18.2 15.2	$C_{43}H_{52}N_{15}O_{22}P_3S_3$	658.582040	0.246	-2	b4
664.811623	507.8	$C_{166}H_{205}N_{60}O_{84}P_{15}S_1$	664.811336	- 0 432	-8	M - 8H
670.551939 677 513599	16.1 13 5	⁵ C ₈₃ H ₁₀₄ N ₂₇ O ₄₄ P ₈ S ₈	670.552651	1.063	-4	c8
685.458267	31.5	$\begin{array}{c} C_{108}H_{134}N_{34}O_{56}P_{10}S_{1}\\ 0\end{array}$	685.458048	- 0.320	-5	b11 - B(dG) - 2H, b11 - B(A) - H2O
685.857091	22.7					
694.810341	110.0	C ₈₈ H ₁₀₉ N ₂₇ O ₄₆ P ₈ S ₈	694.809890	- 0.649	-4	b9 - B(dG) - 2H, b9 - B(A) - H2O
697.056874	7.0	$C_{43}H_{52}N_{16}O_{22}P_4S_4$	697.056494	- 0.546	-2	w4 - H2O
697.548430	7.1	$C_{43}H_{51}N_{15}O_{23}P_4S_4$	697.548501	0.101	-2	w4 - NH3, d4 -
703.619510	13.9	$\begin{array}{c} C_{150}H_{183}N_{54}O_{78}P_{15}S_{1}\\ {}_{5}\end{array}$	703.619697	0.266	-7	d15 - B(T) - NH3, d15 - B(mC) - H2O
706.061275	49.4	C ₄₃ H ₅₄ N ₁₆ O ₂₃ P ₄ S ₄	706.061776	0.710	-2	w4
719.051311	121.0	$C_{22}H_{26}N_8O_{12}P_2S_2$	719.051408	0.135	-1	d2 - H2O, w2 - H2O
719.738330	14.4	$C_{68}H_{86}N_{23}O_{35}P_6S_6$	719.739612	1.781	-3	z7 - B(dA) + 1H
721.198492	49.7	$C_{156}H_{194}N_{50}O_{84}P_{15}S_1$	721.197307	-	-7	M - 7H - 4H - 2d4
724 724901	211		724 735300	1.643	2	$\sqrt{7} = B(dA)$
736.091738	18.6	C681 1851 23 C36F 6 C6	724.755509	0.577	-5	yr D(arty
740.635248	2133.		740.634781	-		M - 7H - 3H -
740 004700	5			0.631		dA
740.901728	12.7					
746.087364	246.2					
752.411435	6.7	$C_{73}H_{90}N_{22}O_{38}P_6S_6$	752.410602	- 1 108	-3	a7 - 2H, b7 - H2O
755.080559	31.7	$C_{48}H_{60}N_{16}O_{25}P_4S_4$	755.080166	-	-2	z5 - B(dA)
759.032567	36.6			0.520		
762.082306	50.2					
763.085669	14.8					
/68.0/545/	19.8	$C_{48}H_{58}N_{18}O_{25}P_4S_4$	/68.0/5415	- 0.054	-2	y5 - B(dC)
769.753990	146.0	$C_{73}H_{90}N_{28}O_{36}P_6S_6$	769.753474	- 0.671	-3	у/
775.384608	19.9			0.071		
784.391943	5.7	$C_{73}H_{91}N_{22}O_{40}P_7S_7$	784.391765	- 0.227	-3	d7 - H2O
801.734667	16.1	$C_{73}H_{91}N_{28}O_{38}P_7S_7$	801.734636	- 0.039	-3	w7
803.051979	15.5	$C_{48}H_{61}N_{16}O_{27}P_5S_5$	803.051909	- 0.087	-2	x5 - B(dA) + 1H, w5 - B(dG)
808.043286	16.6	$C_{47}H_{57}N_{19}O_{26}P_5S_5$	808.043413	0.158	-2	w5 - B(T) - CH3
809.587794	19.2	$C_{53}H_{63}N_{17}O_{27}P_4S_4$	809.588355	0.693	-2	b5 - H2O, a5 - 2H
815.008762	52.2					
816.012031	16.0		047 070004		0	
817.071087	104.0	$C_{78}H_{97}N_{22}O_{42}P_7S_7$	817.070691	- 0 484	-3	2H, b8 - B(A) -
817 100712	17 0		817 308606	-	-3	H2O b8 - B(A) - NH3
017.400742	3.17	O781 1961 №21 O43F 7O7	080080	- 2.503	-0	20 200 100
822.616164	20.5					
823.311133	137.8					

8	830.604221	1243.	$C_{53}H_{65}N_{21}O_{26}P_4S_4$	830.604871	0.782	-2	у5
8	841.566828	4 26.9	$\begin{array}{c} C_{156}H_{194}N_{50}O_{84}P_{15}S_{1}\\ {}_{5}\end{array}$	841.564737	- 2.485	-6	M - 6H - 4H - 2dA
8	842.030939 849.571298	386.4 15.7	$C_{107}H_{132}N_{34}O_{55}P_{10}S_1$	849.571738	0.517	-1 -4	a11 - B(dG) - CH3
8	857.075161	17.3	${\overset{_{0}}{\overset{_{108}}{}}}{\overset{_{108}}{}}{\overset{_{134}}{}}{\overset{_{N_{34}}{}}{}{O_{56}}{\overset{_{P_{10}}}{}}{\overset{_{1}}{}{S_{1}}}$	857.074379	- 0.913	-4	b11 - B(A) - H2O, b11 - B(dG) - 2H
8	862.423395 878.576205 881.731105	13.4 43.4 53.4	$C_{53}H_{66}N_{21}O_{28}P_5S_5$	878.576614	0.465	-2 -3	w5
ģ	905.046742 906.577853	21.1 230.1	$C_{58}H_{70}N_{17}O_{31}P_5S_5$	906.578488	0.700	-2	b6 - B(mC) - H2O, b6 - B(T)
9	917.569871 926.749680	15.9 64.8	$C_{88}H_{109}N_{27}O_{46}P_8S_8$	926.748945	- 0.793	-3	- NH3 b9 - B(A) - H2O, b9 - B(dG) - 2H
	930.590531 940.067833 942.158090	71.8 13.6 24.9		046 502545	0.640	4	712 - B(mC) +
:	940.591909	21.0	U ₁₁₈ Π ₁₄₉ Ν ₄₂ U ₅₉ Ρ ₁₁ U ₁	940.092010	0.040	-4	2H
ę	969.108930	5.3	$C_{63}H_{77}N_{20}O_{32}P_5S_5$	969.107944	- 1.017	-2	a6 - 2H, b6 - H2O
ę	978.113951	7.0	$C_{63}H_{79}N_{20}O_{33}P_5S_5$	978.113226	-	-2	b6
9	980.137463	8.4	$C_{33}H_{37}N_{13}O_{15}P_2S_2$	980.137597	0.741 0.136	-1	y3 - H2O, a3 - 2H, b3 - H2O, z3 - 2H
((996.068657 998.147479 1056.11525	14.2 106.3 14.9	$C_{33}H_{39}N_{13}O_{16}P_2S_2$	998.148162	0.684	-1	b3, y3
	1076.08099 1	7.5	$C_{33}H_{38}N_{13}O_{17}P_3S_3$	1076.08108 5	0.087	-1	d3 - H2O, w3 - H2O
	1091.11730 4	95.8					
	1092.12089 8	36.9					
	2 1094.09104 2	155.4	$C_{33}H_{40}N_{13}O_{18}P_3S_3$	1094.09165 0	0.556	-1	w3, d3
	1129.12030	8.0	$C_{73}H_{90}N_{22}O_{38}P_6S_6$	1129.11954	- 0.676	-2	b7 - H2O, a7 - 2H
	1155.13448	8.4	$C_{73}H_{90}N_{28}O_{36}P_6S_6$	1155.13384	-	-2	у7
	1172.03862	42.9		9	0.540		
	9 1173.04177	14.8					
() 1178.13836	24.8					
	1 1226.11080 2	55.5	$C_{78}H_{97}N_{22}O_{42}P_7S_7$	1226.10967 5	- 0.919	-2	b8 - B(dG) - 2H, b8 - B(A) -
	1266.12333	32.9			-		H2O
	4 1300.16123 5	9.0	$C_{43}H_{50}N_{15}O_{21}P_3S_3$	1300.16079 2	- 0.341	-1	y4 - NH3, a4 - 2H, b4 - H2O
-	1318.17153	73.2	$C_{43}H_{52}N_{15}O_{22}P_3S_3$	1318.17135	-	-1	b4

4			6	0.135		
1413.13035 6	10.6	$C_{43}H_{54}N_{16}O_{23}P_4S_4$	1413.13082 8	0.334	-1	w4
1620.18398 8	8.5	$C_{53}H_{63}N_{17}O_{27}P_4S_4$	1620.18398 6	- 0.001	-1	b5 - H2O, a5 - 2H
1662.21935 7	10.3	$C_{53}H_{65}N_{21}O_{26}P_4S_4$	1662.21701 8	- 1 407	-1	у5
1718.22126 8	30.3		C C			
1719.22524 9	21.2					
1814.16718 3	15.6	$C_{58}H_{70}N_{17}O_{31}P_5S_5$	1814.16425 3	- 1.615	-1	b6 - B(mC) - H2O, b6 - B(T) - NH3
1880.10356 5	8.2					
1894.19319 9	21.2	$C_{118}H_{149}N_{42}O_{59}P_{11}S_{1}$	1894.19230 6	- 0.472	-2	z12 - B(mC) + 2H
1895.19532 5	12.2		-	-		
-			Abs mean error	0.438		
			Abs mean std dev	0.367		

Table S4 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ MALAT-1 by UVPD MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured <i>mz</i>	S/N	Elemental Composition	Theoretical <i>mz</i>	Error (ppm)	Charg e	Assignmen t	
158.925256 165.949398 174.902431 191.965070	16.1 60.0 14.4 26.7		101 065165	0 405	1	c1 - B(dG) -	.11
192.972898 208 890182	48.8 31.3	05116041 0	191.903103	0.490	-1	OCH2	01
317.024071	39.5	$C_{10}H_{13}N_{3}O_{5}PS$	317.024077	0.019	-1	w11(mC)b6 - H2O, w4(mC)b13 - H2O, x1 - OCH2	J2
319.015911	177. 2	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	0.024	-1	x10(T)b7, y10(T)c7, z10(T)d7, b5(T)x12, x7(T)b10, c5(T)y12, a7(T)w10, c7(T)d10, d5(T)z12, a5(T)w12, b7(T)x10, c7(T)y10, d7(T)z10, a10(T)w7, b10(T)x7, c10(T)y7, d10(T)z7, y7(T)c10, d4(T)z13, w7(T)a10, z13(T)d4, x12(T)b5, c4(T)y13, y12(T)c5, w13(T)a4, y13(T)c4, b4(T)x13, x13(T)b4, z12(T)d5, w10(T)a7, y12(T)c5, w13(T)a4, y13(T)c4, b4(T)x13, x13(T)b4, z12(T)d5, w10(T)a7, y12(T)c7, y12(T)c5, w13(T)a4, y13(T)c4, b4(T)x13, x13(T)b4, z12(T)d5, w10(T)a7, y12(T)c7, y12(T)c7, y13(T)c4, b4(T)x13, x13(T)b4, z12(T)d5, w10(T)a7, y12(T)c7, y12(T)c7, y13(T)c4, y13(T)	J3
320.019263 327.019665	19.8 39.6	$C_{10}H_{11}N_5O_4PS$	327.019661	- 0.011	-1	w8(A)b9 - H2O, x5a12, w9(A)b8 - H2O, w6(A)b11 -	J4
328.027496	73.0	$C_{10}H_{12}N_5O_4PS$	328.027486	- 0.032	-1	x5a12 + 1H, a8(A)w9, w9(A)a8, x9(A)b8, y9(A)c8, z9(A)d8, w8(A)a9, y8(A)c9, z8(A)d9, w6(A)a11, x6(A)b11, y6(A)c11, z6(A)d11, b8(A)x9	J5

						c12(G)z5, c8(A)y9, z5(G)c12, d8(A)z9, a9(A)w8, b9(A)x8, c9(A)y8, x8(A)b9, a11(A)w6, b11(A)x6, d9(A)z8, c11(A)y6, a12(G)x5, d11(A)z6	
337.026479	13.7	C ₁₀ H ₁₅ N ₂ O ₇ PS	337.026483	0.010	-1	y13(T)d4 + 2H, y12(T)d5 + 2H, y10(T)d7 + 2H, y7(T)d10 + 2H, b4(T)w13 + 2H, w12(T)b5 + 1H, b5(T)w12 + 2H, b7(T)w10 + 2H, d7(T)y10 + 2H, d10(T)y7 + 2H, w7(T)b10 + 1H, w13(T)b4 + 1H, w10(T)b7 + 1H, d4(T)y13 + 2H, d5(T)w12 + 2H	J6
343.014577	37.6	$C_{10}H_{11}N_5O_5PS$	343.014575	- 0.005	-1	d3(1)y12 + 2H w5b12 - H2O, c1 - OCH2, w6(A)b11 - 2H, w8(A)b9 - 2H, w14(dA)b3 - OCH2, w3(dA)b14 - OCH2, w9(A)b8 - 2H	J7
344.022429	31.7	$C_{10}H_{12}N_5O_5PS$	344.022400	- 0.084	-1	d12(G)z5, x5(G)b12, y5(G)c12, w5(G)a12, y6(A)d11, z5(G)d12, b8(A)w9, y9(A)d8, d8(A)y9, c12(G)y5, b9(A)w8, d9(A)y8, b12(G)x5, a12(G)w5, y8(A)d9, b11(A)w6, d11(A)w6,	J8
346.026822	55.7	C ₁₁ H ₁₄ N ₃ O ₆ PS	346.026817	- 0.014	-1	z15(dC)d2, d2(dC)z15, c2(dC)y15, b2(dC)x15, a2(dC)w15, w15(dC)a2, x15(dC)b2, w1 - H2O, v15(dC)c2	J9
356.022419	75.0	C ₁₁ H ₁₂ N ₅ O ₅ PS	356.022400	- 0.052	-1	b14(dA)x3, z3(dA)d14, d3(dA)z14, w14(dA)a3, a14(dA)w3, c14(dA)y3, y3(dA)c14, x3(dA)b14, x2a15 + 1H, c3(dA)y14,	J1 0

						a15(dG)x2, b3(dA)x14, z2(dG)c15, a3(dA)w14, c15(dG)z2, x14(dA)b3, y14(dA)c3, z14(dA)d3, w3(dA)a14, d14(dA)z3	
356.904043	300. 9					<u> </u>	
364.037375	21.8	$C_{11}H_{16}N_{3}O_{7}PS$	364.037382	0.019	-1	b2(dC)w15 + 2H, d2(dC)y15 + 2H, y15d2 + 2H, w15b2 + 1H, w1	J1 1
372.017416	32.2	C ₁₁ H ₁₂ N ₅ O ₆ PS	372.017315	0.270	-1	z2(dG)d15, w2(dG)a15, d1 - H2O, y3(dA)d14, d3(dA)y14, y14(dA)d3, b3(dA)w14, x2(dG)b15, d15(dG)z2, y2(dG)c15, b14(dA)w3, c15(dG)y2, b15(dG)x2, a15(dG)w2, d14(dA)w3, c15(dG)w2, d15(dG)w2, d14(dA)w3, c15(dG)w2, d14(dA)w3, c15(dG)w2, d14(dA)w3, c15(dG)w2, d14(dA)w3, c15(dG)w2, d14(dA)w3, c15(dG)w2, d14(dA)w3, c15(dG)w2, d14(dA)w3, c15(dG)w2, d	J1 2
390.027876	31.2	$C_{11}H_{14}N_5O_7PS$	390.027880	0.010	-1	d14(dA)y3 d15(dG)y2 + 2H, w2b15 + 1H, y2d15 + 2H, b15(dG)w2 + 2H, d1	J1 3
397.998234 407.993867 413.975373	15.2 40.9 13.0	$C_{10}H_{15}N_{3}O_{7}P_{2}S_{2}$	413.975390	0.041	-1	x4(mC)d13 + 1H, x11(mC)d6 + 1H, w4(mC)c13, w11(mC)c6, d13(mC)x4, c13(mC)x4, c13(mC)x4, d6(mC)x11, c6(mC)w11	J1 4
414.959452 416.841900 418.904458 423.971034	50.4 39.4 89.8 23.3	$C_{10}H_{13}N_5O_6P_2S_2$	423.970973	- 0.145	-1	d9(A)x8, c9(A)w8, c12(G)x5, c8(A)w9, x5(G)c12 + 1H, x6(A)d11 + 1H, d8(A)x9, c11(A)w6,	J1 5
432.970120	15.9	$C_{10}H_{16}N_2O_9P_2S_2$	432.969970	- 0.346	-1	$\begin{array}{l} x8(A)d9 + 1H, \\ d11(A)x6, \\ w9(A)c8, \\ w6(A)c11, \\ x9(A)d8 + 1H, \\ w8(A)c9 \\ d7(T)w10 + 2H, \\ w7(T)d10 + 2H, \\ d10(T)w7 + 2H, \\ d10(T)w7 + 2H, \\ w13(T)d4 + 2H, \\ w13(T)d4 + 2H, \\ w10(T)w13 + 2H, \\ w10(T)d7 + 2H, \\ w12(T)d5 + 2H \end{array}$	J1 6

441.970371	16.2	$C_{11}H_{15}N_3O_8P_2S_2$	441.970304	- 0.153	-1	w15c2, x15d2 + 1H, d2(dC)x15, c2(dC)w15	J1 7
451.965933	24.5	$C_{11}H_{13}N_5O_7P_2S_2$	451.965888	- 0.100	-1	w14(dA)c3, w3(dA)c14, x3(dA)d14 + 1H, x14(dA)d3 + 1H, c15(dG)x2, d14(dA)x3	J1 8
467.960836	23.9	$C_{11}H_{13}N_5O_8P_2S_2$	467.960802	- 0.072	-1	c14(dA)w3, c14(dA)w3, x2(dG)c15 + 1H, d3(dA)w14, c3(dA)w14 x2d15 + 1H, d3(dA)w14, d14(dA)w3, c15(dG)w2, d15(dG)x2, w2(dG)c15, w3(dA)d14, w14(dA)d2	J1 9
469.046360	24.6	$C_{103}H_{127}N_{40}O_{50}P_9S_9$	469.046290	-	-7	y10	
470.054270	17.9	$C_{16}H_{18}N_5O_8PS$	470.054094	0.140 - 0.275	-1	z2 - B(dC) - OCH2	
478.833365 512.996253 522.007742	14.0 51.0 13.4			0.375			
545.534472	13.6	$C_{33}H_{38}N_{13}O_{18}P_3S_3$	545.534362	- 0.201	-2	w3 - 2H, d3 - 2H	
546.542400	12.4	$C_{33}H_{40}N_{13}O_{18}P_3S_3$	546.542187	- 0.389	-2	w3, d3	
585.381633	13.2	$C_{53}H_{66}N_{21}O_{28}P_5S_5$	585.381984	0.600	-3	w5	
586.555417	5.2	$C_{38}H_{44}N_{13}O_{19}P_3S_3$	586.555294	- 0.209	-2	z4 - B(dC) - 2H, y4 - B(T) - NH3, b4 - B(T) - H2O	
601.049458	16.1	$C_{73}H_{91}N_{28}O_{38}P_7S_7$	601.049158	- 0.499	-4	w7	
638.055123	27.1			0.100			
641.118702	21.0	$C_{22}H_{27}N_8O_{11}PS$	641.118485	- 0.339	-1	b2, y2	
645.737182	14.0	$C_{63}H_{77}N_{20}O_{32}P_5S_5$	645.736204	- 1.514	-3	b6 - H2O, a6 - 2H	
647.804911	23.9	$C_{161}H_{199}N_{55}O_{84}P_{15}S_{1}$	647.803546	- 2.108	-8	M - 8H - 4H - dA	
657.062398	14.4	Č ₁₄₄ H ₁₇₉ N ₅₂ O ₇₂ P ₁₃ S ₁	657.062754	0.542	-7	y14, b14	
663.061700	12.1	5					
664.686358	947.	$C_{166}H_{204}N_{60}O_{84}P_{15}S_1$	664.685358	-	-8	M - 8H - 4H	
672.049124	3 10.5	${\overset{_{5}}{C}}_{103}H_{123}N_{40}O_{51}P_{10}S_{1}$	672.049607	1.504 0.719	-5	x10 - 4H	
673.057134	10.8	$^{0}C_{103}H_{128}N_{40}O_{51}P_{10}S_{1}$	673.057432	0.443	-5	x10 + 1H	
676.256468	33.9	$^{0}C_{103}H_{128}N_{40}O_{52}P_{10}S_{1}$	676.256415	-	-5	w10	
683.558773	18.4	${\overset{_{0}}{C}}{_{128}}H_{159}N_{44}O_{65}P_{12}S_{1}$	683.559204	0.630	-6	a13 - B(mC)	
689.559898 695.060777	22.4 8.1	² C ₆₃ H ₇₈ N ₂₆ O ₃₂ P ₆ S ₆	695.060238	- 0.776	-3	w6	
703.074287 706.061369 712.669882	26.9 54.4 12.8	$C_{43}H_{54}N_{16}O_{23}P_4S_4$	706.061776	0.576	-2	w4	

719.051272	20.1	$C_{22}H_{26}N_8O_{12}P_2S_2$	719.051408	0.190	-1	d2 - H2O, w2 - H2O
728.573632	10.2	$C_{93}H_{114}N_{32}O_{46}P_8S_8$	728.573513	- 0 163	-4	b9 - H2O, a9 - 2H
737.062121	16.5	$C_{22}H_{28}N_8O_{13}P_2S_2$	737.061973	- 0.201	-1	w2, d2
740.064886	6.8	$C_{113}H_{142}N_{43}O_{57}P_{11}S_1$	740.064251	- 0.858	-5	w11
740.492052	70.3	['] C ₁₆₁ H ₁₉₉ N ₅₅ O ₈₄ P ₁₅ S ₁	740.490806	- 1.683	-7	M - 7H - 4H - dA
752.074736	40.1	$C_{48}H_{62}N_{12}O_{28}P_4S_4$	752.074215	- 0.693	-2	b5 - B(dA) + 2H
754.463203	11.0	C ₁₁₈ H ₁₄₆ N ₃₉ O ₆₁ P ₁₁ S ₁ 1	754.463983	1.034	-5	y12 - B(A) - NH3, b12 - B(G) - 2H, b12 - B(A) - H2O
759.784521	80.0	$C_{166}H_{204}N_{60}O_{84}P_{15}S_1$	759.784305	- 0.284	-7	M - 7H - 4H
763.750391	13.2	C ₇₃ H ₈₈ N ₂₈ O ₃₅ P ₆ S ₆	763.749952	- 0.575	-3	z7 - 2H, y7 - H2O
781.274362	36.5	$C_{123}H_{152}N_{45}O_{60}P_{11}S_1$	781.278079	4.758	-5	z12 - 2H, y12 - H2O
801.734371 804.069509	17.5 9.6	C ₇₃ H ₉₁ N ₂₈ O ₃₈ P ₇ S ₇ C ₁₂₃ H ₁₅₅ N ₄₅ O ₆₃ P ₁₂ S ₁ 2	801.734636 804.068889	0.330 - 0.771	-3 -5	w7 w12
808.327478 809.589322	25.6 25.1	$C_{53}H_{63}N_{17}O_{27}P_4S_4$	809.588355	- 1.195	-2	b5 - H2O, a5 - 2H
817.010652 821.600798	23.2 8.4	$C_{53}H_{63}N_{21}O_{25}P_4S_4$	821.599588	- 1 /172	-2	y5 - H2O, z5 - 2H
830.605343	5.9	$C_{53}H_{65}N_{21}O_{26}P_4S_4$	830.604871	- 0.568	-2	y5
842.030972 845.483803 849.571789	26.5 10.6 9.5	$C_{107}H_{132}N_{34}O_{55}P_{10}S_1$	849.571738	-	-4	a11 - B(dG) -
861.753172	14.3	0		0.060		CH3
864.073179	20.0	C ₁₆₁ H ₁₉₉ N ₅₅ O ₈₄ P ₁₅ S ₁ 5	864.073820	0.742	-6	M - 6H - 4H - dA
866.566024	7.2	$C_{53}H_{66}N_{17}O_{30}P_5S_5$	866.565381	- 0.742	-2	d5
873.428024	9.4	$C_{83}H_{100}N_{33}O_{39}P_7S_7$	873.428206	0.208	-3	z8 - 2H, y8 - H2O
878.576005 886.581952	15.9 104. 1	$\begin{array}{c} C_{53}H_{66}N_{21}O_{28}P_5S_5\\ C_{166}H_{204}N_{60}O_{84}P_{15}S_1\\ 5\end{array}$	878.576614 886.582902	0.693 1.072	-2 -6	w5 M - 6H - 4H
906.578071	7.7	$C_{58}H_{70}N_{17}O_{31}P_5S_5$	906.578488	0.460	-2	b6 - B(mC) - H2O, b6 - B(T) - NH3
911.747433 926.749561	15.0 5.2	C ₈₃ H ₁₀₄ N ₃₃ O ₄₂ P ₈ S ₈ C ₈₈ H ₁₀₉ N ₂₇ O ₄₆ P ₈ S ₈	911.748832 926.748945	1.535 - 0.665	-3 -3	w8 + 1H b9 - B(A) - H2O, b9 - B(dG) - 2H
968.604133 969.108598	20.1 17.6	$C_{63}H_{77}N_{20}O_{32}P_5S_5$	969.107944	- 0.675	-2	a6 - 2H, b6 - H2O
972.101125 976.592047	13.5 9.2	C ₁₂₃ H ₁₄₉ N ₄₄ O ₆₁ P ₁₁ S ₁ 1	976.591509	- 0.551	-4	a12 - 4H
977.085164 983.105901	19.1 9.1	$C_{93}H_{112}N_{38}O_{43}P_8S_8$	983.106460	0.568	-3	z9 - 2H, y9 -

986.117343	8.7	$C_{63}H_{75}N_{26}O_{29}P_5S_5$	986.116969	-	-2	H2O y6 - H2O, z6 - 2H
995.122638	15.1	$C_{63}H_{77}N_{26}O_{30}P_5S_5$	995.122252	-	-2	y6
998.148057 1023.07981	17.6 10.5	$C_{33}H_{39}N_{13}O_{16}P_2S_2$	998.148162	0.388	-1	b3, y3
1037.68925 6	9.0					
1043.09456 9	5.1	$C_{63}H_{78}N_{26}O_{32}P_6S_6$	1043.09399 5	- 0.550	-2	w6
1060.10369 7	26.7					
1061.10687 7	9.4					
1094.09091 1	42.6	$C_{33}H_{40}N_{13}O_{18}P_3S_3$	1094.09165 0	0.676	-1	w3, d3
1128.61629 8	10.3					
1129.11959 3	23.7					
1226.10927 1	9.7	$C_{78}H_{97}N_{22}O_{42}P_7S_7$	1226.10967 5	0.329	-2	b8 - B(dG) - 2H, b8 - B(A) - H2O
1300.16035 1	6.7	$C_{43}H_{50}N_{15}O_{21}P_3S_3$	1300.16079 2	0.339	-1	y4 - NH3, a4 - 2H, b4 - H2O
1317.18722 0	18.7	$C_{43}H_{53}N_{16}O_{21}P_3S_3$		0.092	-1	y4
1318.19061 9	8.5					
1413.13066 3	8.1	$C_{43}H_{54}N_{16}O_{23}P_4S_4$	1413.13082 8	0.117	-1	w4
			Abs mean error	0.654		
			Abs mean std dev	0.771		

Table S5 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ danvatirsen by EDD MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured <i>mz</i>	S/N	Elemental Composition	Theoretical <i>mz</i>	Error (ppm)	Charg e	Assignmen t	
318.008280	90.6	C ₁₀ H ₁₂ N ₂ O ₆ PS	318.008093	- 0.590	-1	$\begin{array}{c} y4d13 - NH2,\\ y5(T)c12 - 1H,\\ z5(T)d12 - 1H,\\ x5(T)b12 - 1H,\\ w4b13 - NH3,\\ w7(T)b10 -\\ H2O, d4(T)z13 -\\ 1H, d6(T)z11 -\\ 1H, c4(T)y13 -\\ 1H, c5(T)y12 -\\ 1H, d5(T)z12 -\\ 1H, d6(T)x11 -\\ 1H, b6(T)x11 -\\ 1H, b6(T)x11 -\\ 1H, b6(T)x11 -\\ 1H, b6(T)y11 -\\ 1H, a5(T)w12 -\\ 1H, a7(T)b10 -\\ 1H, a7(T)b10 -\\ 1H, w5(T)b12 -\\ H2O, y7(T)c10 -\\ 1H, z7(T)d10 -\\ 1H, z7(T)d10 -\\ 1H, b5(T)x12 -\\ 1H \\ \end{array}$	J 1
319.016114	99.6	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	- 0.610	-1	a5(T)w12, a4(T)w13, b4(T)x13, c4(T)y13, d4(T)z13, w4b13 - NH2, z5(T)d12, b5(T)x12, x5(T)b12, y5(T)c12, d6(T)z11, c5(T)y12, w7(T)a10, d5(T)z12, a6(T)w11, b6(T)x11, y7(T)c10, z7(T)d10, w5(T)a12, w7(J 2
327.019835	17.7	$C_{10}H_{11}N_5O_4PS$	327.019661	- 0.530	-1	x7(1)b10 w8b9 - H2O, x8(A)b9 - 1H, z6(G)c11 - 1H, c8(G)29 - 1H, a8(G)x9 - 1H, y8(A)c9 - 1H, z8(A)d9 - 1H, c7(G)z10 - 1H, a7(G)x10 - 1H, x6a11, b9(A)x8 - 1H, w8(A)a9 - 1H, a9(A)w8 - 1H	J 3
328.027641	18.4	$C_{10}H_{12}N_5O_4PS$	328.027486	- 0.470	-1	z6(G)c11, y8(A)c9, c8(G)29, a8(G)x9, c7(G)z10, a7(G)x10,	J 4

							a9(A)w8, x8(A)b9, w8(A)a9, b9(A)x8, z8(A)d9	
	328.027641	18.4	$C_{10}H_{11}N_5O_4PS$	328.027486	0.470	-1		
	343.014692	115.7	$C_{10}H_{11}N_5O_5PS$	343.014575	- 0.340	-1	w6b11 - H2O, d7(G)z10 - 1H, c7(G)y10 - 1H, z6(G)d11 - 1H, b7(G)x10 - 1H, a7(G)w10 - 1H, d8(G)z9 - 1H, x6(G)b11 - 1H, y6(G)c11 - 1H, w8b9 - 2H, y8(A)d9 - 1H,	J 5
	344.022520	58.5	$C_{10}H_{12}N_5O_5PS$	344.022400	- 0.350	-1	w6(G)a11 - 1H, a8(G)w9 - 1H, b9(A)w8 - 1H, b8(G)x9 - 1H, c8(G)y9 - 1H, b9(A)w8, w6(G)a11, d8(G)z9, c8(G)y9, b8(G)x9, a8(G)w9, c7(G)y10, b7(G)x10, d7(G)z10, a7(G)w10, x6(G)b11, y8(A)d9, y6(G)c11, z6(G)d11, w8b9 - 1H	J 6
	344.022520	58.5	$C_{10}H_{11}N_5O_5PS$	344.022400	0.350	-1	wobo III	
	361.026609	16.0	$C_{12}H_{14}O_7N_2PS$	361.026482	- 0.350	-1	w1 - NH3, d1 - NH3	
	370.038056	21.2	C ₁₂ H ₁₄ N ₅ O ₅ PS	370.038050	- 0.020	-1	c3(dA)y14, a3(dA)w14, w3(dA)a14, y3(dA)c14, z2(dG)c15, b3(dA)x14, z3(dA)a14, x3(dA)b14, d3(dA)z14	J 7
	370.038056	21.2	$C_{12}H_{13}N_5O_5PS$	370.038050	0.020	-1		
	378.053049	31.4	$C_{12}H_{17}O_7N_3PS$	378.053032	-	-1	a 1, W1	
	398.982245	31.3	$C_0H_7N_0O_4P_2S$	398,982243	0.040	-1		
	409.522859	60.2	$C_{21}H_{38}N_4O_{16}P_7$	409.522856	0.010	-2		
	414.959337	18.1	$C_8H_{13}N_5O_5P_4S$	414.959336	0.000	-1		
	414.959337	18.1	C ₁₀ H ₁₄ N ₂ O ₈ P ₂ S ₂	414.959405	0.160	-1	c6(1)w11, d4(T)x13, d6(T)x11, c4(T)w13, w7(T)c10, c5(T)w12, d5(T)x12, w5(T)c12	J 8
	423.988646	18.2	$C_7H_{17}N_6O_5PS_4$	423.988638	0.020	-1		
	432.969837	23.6	$C_{21}H_{10}N_2OPS_3$	432.969837	0.000	-1 1		
	450.004224	۲۲.9 62	$C_7 \Pi_{19} \Pi_9 O_2 \Pi_3 O_3$ $C_9 \Pi_9 \Pi_9 O_2 \Pi_3 O_3 O_2 \Pi_3 O_2 \Pi_3 O_2 \Pi_3 O_3 O_2 \Pi_3 O_3 O_3 O_3 O_3 O_3 O_3 O_3 O_3 O_3 O$	450.004219	0.010	-1 -2		
	472.094704	15.8	$C_8H_7N_{23}OP$	472.094703	0.000	-1		
	484.387762	26.4	C ₄₆ H ₅₇ N ₁₆ O ₂₃ P ₄ S ₄	484.387742	-	-3	w4	
	404 50000-				0.040	•		
-	491.530627	6.6	C ₃₃ H ₆₇ N ₂	491.530974	0.710	-2		

512.995973	33.8	$C_5H_3N_{22}O_3P_2S$	512.995991	0.040	-1	
554.558438	46.6	C ₃₆ H ₄₄ O ₁₉ N ₁₀ P ₃ S ₃	554.558508	0.130	-2	d3 - 3H
567.565546	8.6	C ₃₆ H ₄₄ O ₁₈ N ₁₃ P ₃ S ₃	567.565662	0.200	-2	w3
591.061951	23.4	$C_{56}H_{70}N_{18}O_{29}P_5S_5$	591.062140	0.320	-3	w5
595.075252	3.9	$C_{41}H_{40}N_{10}O_{20}P_3S_3$	595.075528	0.460	-2	y4 - B(dG) -
0001010202	0.0		0001010020		-	NH3, b4 - B(T)
						- H2O, a4 -
600 200002	40 E		600 200004	0 000	4	B(1) w7
609.308003	48.5	$C_{76}H_{94}N_{25}O_{40}P_7S_7$	609.308004	0.000	-4	VV /
639.038898	18.5	$C_{29}H_{20}N_7OP_3S_2$	639.038910	0.020	-1	
647.548037	3.0	$C_{41}H_{53}N_7O_{25}P_4S_4$	647.547044	-	-2	04 - B(0A)
				1.530		
651.407623	9.6	$C_{66}H_{79}N_{16}O_{34}P_5S_5$	651.408424	1.230	-3	a6 - 4H
651.744473	24.8	$C_{66}H_{80}N_{16}O_{34}P_5S_5$	651.744548	0.110	-3	b6 - H2O, a6
652.406790	2.9	$C_{36}H_{64}NO_3P_2S$	652.408764	3.030	-1	
652.409297	2.9	$C_{66}H_{80}N_{15}O_{35}P_5S_5$	652.408495	-	-3	b6 - NH2
				1.230		
657.593024	115.5	$C_{46}H_{54}N_{12}O_{22}P_3S_3$	657.593080	0.080	-2	a4 - 3H
658.097096	47.3	$C_{46}H_{55}N_{12}O_{22}P_3S_3$	658.096992	-	-2	b4 - H2O, a4
				0.160		
658.591164	12.1	$C_{46}H_{54}N_{11}O_{23}P_3S_3$	658.589274	-	-2	b4 - NH3
				2.870		
660.819049	16.9		660.819337	0.440	-4	a8 - 5H
664 045342	47.0	$C_{40}H_{20}N_{40}O_{44}P_{4}$	664 045342	0.000	-1	
668 087356	4 0	$C_{10}H_{20}N_{10}O_{10}H_{2}$	668 087348	-	-3	z6. v6 - H2O
000.007000	4.0		000.007040	0.010	-0	,,
668 551047	15		668 551005	0.010	2	
674 067670	4.0		674 067672	0.070	-2	M - 8H - H2O
074.007070	13.2	$C_{172}\Pi_{207}\Pi_{56}O_{87}P_{15}O_{15}$	0/4.00/0/3	0.000	-0	M - 011 - 1120
676 217002	5100		676 219004	1 610	o	M - 8H
070.317903	010Z.	$C_{172}\Pi_{209}\Pi_{56}O_{88}\Pi_{15}O_{1}$	070.310994	1.010	-0	
070 040400	ა 400.4		070 040400	0.040	4	
676.940402	402.1	$C_4H_{10}N_{23}O_5P_7$	676.940408	0.010	-1	
681.057404	14.4	$C_{106}H_{129}N_{33}O_{57}P_{10}S_{1}$	681.056526	-	-5	u IU - 0H
				1.290	•	
682.225587	12.7	$C_{126}H_{153}N_{44}O_{66}P_{12}S_1$	682.225114	-	-6	W12 - 7H
		2		0.690	_	
682.724923	3.1	$C_3H_8N_4O_{17}P_9S$	682.724923	0.000	-2	
690.863221	18.7	$C_{106}H_{128}N_{40}O_{54}P_{10}S_1$	690.862316	-	-5	w10 - 6H
		0		1.310		
691.262475	10.1	$C_{29}H_{43}N_{10}O_4S_3$	691.263637	1.680	-5	
691.566315	5.8	C ₂₇ H ₇₇ N ₁₄ P ₂ S	691.565707	0.880	-2	
691.566556	24.5	C ₈₆ H ₁₀₆ N ₃₀ O ₄₄ P ₈ S ₈	691.566694	0.200	-4	w8
692.315180	5.5	C ₂₃ H ₆₄ N ₆ O ₃ P ₄ S ₃	692.315800	0.900	-2	
695.562624	17.4	C ₃₇ H ₈₁ N ₂ O ₅ P ₂	695.562621	0.000	-2	
706.071190	5.1	$C_{48}H_{20}OP_{2}S$	706.071559	0.520	-1	
706.071868	12.9	C ₆₆ H ₈₂ N ₂₃ O ₃₄ P ₆ S ₆	706.072032	0.230	-3	w6
715.073812	5.7	$C_{46}H_{58}N_{12}O_{25}P_4S_4$	715.074018	0.290	-2	d4
721.022577	12.4	$C_{22}HN_{25}O_2P_2$	721.022577	0.000	-1	
721 022740	4 1	CraHarNacOpPcS	721 022667	0 100	-2	
727 085199	32.6	C_{14} H_{2} H_{19} C_{31} R_{6}	727 085251	0.070	-2	w4
735 206725	31	$C_{46} H_{58} + G_{6} + O_{23} H_{40} + O_{23} + A_{23} + A_{23}$	735 207567	1 150	-7	w15. d15
100.200120	0.1	-	100.201001	1.100	•	-, -
710 086171	20 5		7/0 086701	0 120	_1	d2
7/3 07010/	20.0		712 070101	0.430	-1	a9 - 5H
143.019104	04.9	0961 1114 N31 048 P808	143.010104	-	-4	
740 577455	10.4		740 570404	1.270	4	60 NU2
143.511455	19.4	U96H114N30U49P8S8	143.516124	-	-4	פטאו - פט
7/7 0007 10	44.0		747 0007 10	1.790	•	
/4/.082548	11.3	$C_{22}H_{54}NO_2PS_{11}$	/4/.082548	0.000	-6	0 0 1/00
749.335613	10.7	$C_{96}H_{115}N_{35}O_{46}P_8S_8$	749.335600	-	-4	z9, y9 - H2O
				0.020		
754.214385	2.2	$C_{29}H_{62}NOP_6S_4$	754.214546	0.210	-1	

754.867596	5.3	$C_{116}H_{141}N_{42}O_{60}P_{11}S_1$	754.866955	- 0.850	-5	w11 - 6H
765 002008	27.2		765 002272	0.000	1	w2
705.095000	Z1.3 E1.0	$C_{24}\Pi_{31}O_{13}\Pi_8\Gamma_2O_2$	705.095275	0.350	-1	w∠ o7 /⊔
100.419021	51.0	$C_{76}\Pi_{91}\Pi_{21}O_{39}\Pi_{6}O_{6}O_{6}$	700.410499	-	-3	a <i>i</i> - 411
770 700400	<u> </u>		770 700047	1.470	7	
//2./92196	62.6	$C_{172}H_{208}N_{56}O_{88}P_{15}S_1$	//2./9201/	-	-1	IVI - 9H
		5		0.230		
774.761375	9.7	$C_{76}H_{92}N_{25}O_{37}P_6S_6$	774.761746	0.480	-3	y7 - H2O, z7
777.573379	20.3	$C_{96}H_{117}N_{35}O_{49}P_9S_9$	777.572294	-	-4	w9 - 5H
				1.400		
791.276961	55.7	$C_{126}H_{151}N_{40}O_{65}P_{11}S_1$	791.276290	-	-5	a12 - 6H
		1		0.850		
804.739265	8.0	C76H95N21O42P7S7	804.739124	-	-3	d7
		- 10 33 21 - 72 1 1		0 180		
812 411861	33.1	C==H=+N==O+=P=S=	812 410672	-	-3	w7 - 4H
012.411001	00.1		012.410072	1 /60	0	
010 100071	17 0		010 100001	0.010	1	
010.100074	17.0	$C_{41}\Pi_{36}\Pi_{5}\Gamma_{4}O_{3}$	010.100001	0.010	-1	w12 6H
818.872474	122.4	$C_{126}H_{154}N_{44}O_{66}P_{12}S_{1}$	818.87 1593	-	-5	W12 - 011
	. – .	2		1.080		
823.085037	17.3	$C_{106}H_{127}N_{33}O_{54}P_9S_9$	823.083963	-	-4	a10 - 5H
				1.300		
823.583285	5.5	$C_{106}H_{127}N_{32}O_{55}P_9S_9$	823.581923	-	-4	b10 - NH3
				1.650		
829.617160	3.5	$C_{56}H_{67}N_{18}O_{26}P_4S_4$	829.616184	-	-2	z5 - 3H
				1.180		
830,119776	35.3		830,119822	0.060	-2	y5 - H2O, z5
833 120823	17 7	$C_0H_0N_{40}O_4PS$	833 120823	0.000	-1	-
835 593028	72	C_{4}	835 593020	-	_4	z10. v10 - H2O
000.000020	1.2		000.000020	0.010	-7	,
020 011001	0.5		020 012011	0.010	1	v10 - 5H
039.044904	9.5	C ₁₀₆ I ₁₂₈ N ₄₀ O ₅₂ F ₉ O ₉	039.043041	-	-4	yro on
054 000000	4.0		054 004005	1.300	4	d10
851.823838	4.8	$C_{106}H_{131}N_{33}O_{57}P_{10}S_{1}$	851.824295	0.540	-4	uiu
		0			_	40.011
855.084521	4.4	$C_{136}H_{165}N_{43}O_{70}P_{12}S_1$	855.084125	-	-5	a13 - 6H
		2		0.460		
858.092009	16.8	C ₁₉ H ₁₈ N ₂₈ O ₆ P ₄	858.092007	0.000	-1	
858.092103	3.7	$C_{25}H_{22}N_{25}P_6$	858.092121	0.020	-2	
860.086105	116.5	C ₁₃₆ H ₁₆₄ N ₄₆ O ₆₉ P ₁₂ S ₁	860.085422	-	-5	z13 - 6H
		2		0.790		
861.886908	2.6	C105H180N43O88P14S1	861.887187	0.320	-5	
	-	- 100 100 - 0- 00 14 1			-	
863 830516	73		863 829713	-	-4	w10 - 5H
000.000010	1.0		000.0207 10	0 030		
875 085776	37		875 085880	0.000	2	d5
013.003110	20.7		073.003009	0.150	-2	a8 - 1H
001.429/10	30.3	$C_{86}\Pi_{103}\Pi_{26}O_{44}P_7S_7$	001.420391	-	-3	au - 411
000 00 4000	0.4		000 00000	1.500	0	
882.094080	8.4	$C_{86}H_{103}N_{25}O_{45}P_7S_7$	882.092338	-	-3	DO - INH3
				1.980		
884.440693	48.1	C ₈₆ H ₁₀₄ N ₃₀ O ₄₁ P ₇ S ₇	884.440183	-	-3	y8 - H2O, z8
				0.580		
885.105249	8.4	C ₈₆ H ₁₀₄ N ₂₉ O ₄₂ P ₇ S ₇	885.104130	-	-3	y8 - NH2
				1.260		
887.096956	35.8	$C_{56}H_{71}N_{18}O_{29}P_5S_5$	887.096848	-	-2	w5
				0.120		
899 094468	42		899 092747	-	-6	M - 6H - H2O
		5	500.00E1 11	1 910	-	
901 591283	71 5		901 590596	-	-6	M - 9H
001.001200	71.0	- -	001.000000	0 760	-0	
001 758566	7/1		001 758566	0.700	-6	M - 8H
301.730300	14.1	U1721 12091 156U88F15O1	301.730300	0.000	-0	
		5				

905.589165	11.2	C ₃₂ H ₇₈ N ₁₈ O ₁₀ P	905.589141	0.030	-1	we 002112
908.419775 909.341954	2.4 16.2	$C_{84}H_{105}N_{30}O_{43}P_8S_8$ $C_{116}H_{139}N_{38}O_{59}P_{10}S_1$	908.421163 909.341382	- - 0.630	-3 -4	a11 - 5H
915.348509	8.6	$C_{116}^{0}H_{139}N_{42}O_{57}P_{10}S_{1}$	915.346999	- 1.650	-4	z11 - 5H
922.425147	28.0	°C ₈₆ H ₁₀₇ N ₃₀ O ₄₄ P ₈ S ₈	922.424867	- 0.300	-3	w8
943.836734	9.0	$C_{116}H_{142}N_{42}O_{60}P_{11}S_{1}$	943.835512	- 1.290	-4	w11 - 5H
977.618677	15.1	$C_{66}H_{80}N_{16}O_{34}P_5S_5$	977.616548	- 2.180	-2	a6 - 3H
989.347530	13.2	$C_{126}H_{152}N_{40}O_{65}P_{11}S_{1}$	989.347181	- 0.350	-4	a12 - 5H
991.107124	30.9	$C_{96}H_{115}N_{31}O_{48}P_8S_8$	991.106645	- 0.480	-3	a9 - 4H
991.442065	40.5	$C_{96}H_{116}N_{31}O_{48}P_8S_8$	991.442404	0.340	-3	b9 - H2O, a9
999.448856	11.1	C ₉₆ H ₁₁₆ N ₃₅ O ₄₆ P ₈ S ₈	999.449893	1.040	-3	y9 - H2O, z9
1002.13093 6	12.8	$C_{66}H_{79}N_{23}O_{31}P_5S_5$	1002.13102 2	0.090	-2	z6 - 3H
1037.10043 0	9.8	$C_{96}H_{118}N_{35}O_{49}P_9S_9$	1037.09881 8	- 1.550	-3	w9 - 4H
1040.19583 6	3.0	$C_{36}H_{44}O_{16}N_{13}P_2S_2$	1040.19566 1	- 0.170	-1	у3
1059.61267 1	9.1	$C_{66}H_{83}N_{23}O_{34}P_6S_6$	1059.61196 1	- 0.670	-2	w6
1075.11034 7	6.3	$C_{71}H_{88}N_{16}O_{38}P_6S_6$	1075.11032 0	- 0.030	-2	b7 - B(G) - H2O, a7 - B(G)
1136.13861 8	22.5	$C_{36}H_{45}O_{18}N_{13}P_3S_3$	1136.13860 0	- 0.020	-1	w3
1150.13424 3	7.4	$C_{76}H_{92}N_{21}O_{39}P_6S_6$	1150.13138 6	- 2.480	-2	а7 - 3Н
1219.62452 2	12.0	$C_{76}H_{96}N_{25}O_{40}P_7S_7$	1219.62355 8	- 0.790	-2	w7
1317.20236 9	9.3	$C_{46}H_{56}N_{12}O_{22}P_3S_3$	1317.20181 0	- 0.420	-1	b4 - H2O, a4
			Abs mean error	0.770		
			Abs mean std dev	0.671		

Table S6 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ danvatirsen by CID MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured <i>mz</i>	S/N	Elemental Composition	Theoretical <i>mz</i>	Error (ppm)	Charg e	Assignmen t	
319.016302	16.9	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	- 1.200	-1	a5(T)w12, a4(T)w13, b4(T)x13, c4(T)y13, d4(T)z13, w4b13 - NH2, z5(T)d12, b5(T)x12, x5(T)b12, y5(T)c12, d6(T)z11, c5(T)y12, w7(T)a10, d5(T)z12, a6(T)w11, c6(T)y11, b6(T)x11, y7(T)c10, z7(T)d10, w5(T)a12, x7(T)b10	J 1
337.026752 344.022589	22.2 97.6	$C_5H_{11}N_{10}O_2P_2S$ $C_{10}H_{12}N_5O_5PS$	337.026788 344.0224	0.110 - 0.550	-3 -1	b9(A)w8, w6(G)a11, d8(G)z9, c8(G)y9, b8(G)x9, a8(G)w9, c7(G)y10, b7(G)x10, d7(G)z10, a7(G)w10, x6(G)b11, y8(A)d9, y6(G)c11, z6(G)d11, w8b0 1H	J 2
344.022589 359.999701 361.026451	97.6 17.0 20.5	C ₅ H ₈ N ₁₃ P ₂ S C ₁₅ H ₆ NO ₁₀ C ₁₂ H ₁₄ O ₇ N ₂ PS	344.022706 359.999719 361.026482	0.340 0.050 0.090	-1 -1 -1	w1 - NH3, d1 -	
369.539755	1044.	$C_{24}H_{31}O_{14}N_5P_2S_2\\$	369.539757	0.010	-2	NH3 d2	
370.038087	803.4	$C_{12}H_{14}N_5O_5PS$	370.03805	- 0.100	-1	c3(dA)y14, a3(dA)w14, w3(dA)a14, y3(dA)c14, z2(dG)c15, b3(dA)x14, z3(dA)d14, x3(dA)b14, d3(dA)z14	J 3
378.041426	19.5	$C_{36}H_{43}O_{18}N_{13}P_3S_3$	378.041349	- 0 200	-3	w3	
378.053060	20.1	$C_{12}H_{17}O_7N_3PS$	378.053032	-	-1	d1, w1	
414.959683	143.4	$C_{10}H_{14}N_2O_8P_2S_2$	414.959405	- 0.670	-1	c6(T)w11, d4(T)x13, d6(T)x11, c4(T)w13, w7(T)c10, c5(T)w12, d5(T)w12,	J 4

						w5(T)c12
442.059229	134.0	$C_{14}H_{23}NO_9P_3$	442.059116	0.260	-1	
476.380460	18.8	$C_{46}H_{57}N_{12}O_{25}P_4S_4$	476.380253	-	-3	d4
		- +0 57 12 - 25 + +		0 430		
484 387972	145.0	CueHNueOeePuSu	484 387742	-	-3	w4
404.007072	140.0	0461 15/1016 0231 404	404.007742	0 / 80	0	
107 015010	16.6		407 044040	0.400	F	w7
407.240040	40.0	$C_{76}\Pi_{93}\Pi_{25}O_{40}\Pi_{7}O_{7}O_{7}O_{7}O_{7}O_{7}O_{7}O_{7}O$	407.244940	-	-5	VV /
	/		404 50005	0.210	•	
491.530667	55.1	$C_{24}H_{44}NO_{30}P_3S_2$	491.53067	0.010	-2	
494.985108	88.0	C ₁₀ H ₄ N ₁₄ O ₇ PS	494.98512	0.030	-1	
500.043990	30.3	$C_2H_5N_{27}P_3$	500.043958	0.060	-2	
507.090852	79.9	$C_{36}H_{44}O_{17}N_{10}P_2S_2$	507.090677	-	-2	b3
				0.350		
512 996265	503 1	$C_2H_2N_{20}O_2PS_2$	512 996371	0 210	-1	
519 593932	79.5	C_{3}	519 593918	-	-2	v3
010.000002	10.0		010.000010	0 030	2	,
520 002026	E10 0		520 002052	0.050	1	
536.002620	040.Z	$C_3 \Pi_5 N_{23} O_5 \Gamma S_2$	536.002655	0.050	-1	
545.054238	18.1	$C_{33}H_5N_8O_2$	545.054095	0.260	-1	
545.055739	12.1	$C_{32}H_{21}OP_4$	545.054837	1.650	-2	
553.051453	38.0	C ₈₆ H ₁₀₅ N ₃₀ O ₄₄ P ₈ S ₈	553.0519	0.810	-5	w8
558.559663	68.2	C ₃₆ H ₄₂ O ₁₇ N ₁₃ P ₃ S ₃	558.56038	1.280	-2	x3 - 3H, w3 -
						H2O
561.104992	9.2	$C_{40}H_{18}O_2P$	561.10499	0.000	-1	
567.565418	614.7	C ₃₆ H ₄₄ O ₁₈ N ₁₃ P ₃ S ₃	567.565662	0.430	-2	w3
571.545809	12.0	$C_{33}H_{72}N_4OP$	571.544924	1.550	-4	
578.042940	17.9	$C_{71}H_{87}N_{22}O_{30}P_7S_7$	578.043276	0.580	-4	w7 - B(mC)
579 316507	8.6	$C_{r_2}H_{00}N_{40}O_{74}P_7$	579 31607	0 750	-2	. ,
570 316876	31.2		570 316515	0.100	1	b7
575.510070	51.2	0761 1931 121 0401 606	573.510515	-	-4	
505 000044	0.0		505 000400	0.020		
585.322011	9.8	$C_{76}H_{93}N_{25}O_{38}P_6S_6$	585.322132	0.210	-4	y/
586.112564	43.6	$C_{17}H_{19}N_{17}O_2P_3$	586.112598	0.060	-1	
588.520297	19.7	$C_{31}H_{62}N_{11}$	588.519515	1.330	-1	
591.062123	41.4	$C_{56}H_{70}N_{18}O_{29}P_5S_5$	591.06214	0.030	-3	w5
598.799595	439.5	C ₇₆ H ₉₂ N ₂₁ O ₄₁ P ₇ S ₇	598.799746	0.250	-4	d7 - H2O, c7 -
						5H
606.546232	16.3	C ₁₁₁ H ₁₃₆ N ₃₇ O ₆₀ P ₁₁ S ₁	606.546713	0.790	-6	w11 - B(A)
		1				
607.473110	7.8	$C_{131}H_{157}N_{44}O_{68}P_{13}S_1$	607.47395	1.380	-7	x13 - B(T) -
		3				H2O
609.306996	855.9		609.308004	1.650	-4	w7
611 118205	99	$C_{47}H_{24}N_{4}O_{40}S_{2}$	611 118197	0.010	-1	
617 080807	6.0	$C_{17}H_{3}H_{4}C_{16}C_{2}$	617 080001	0.010	_2	
622 056957	166		622 057025	1 570	-2	wΩ
022.000007	10.0	С ₉₆ П ₁₁₇ N ₃₅ О ₄₉ Р ₉ S ₉	022.007000	1.570	-5 7	410
626.909298	27.6	$C_{136}H_{167}N_{43}O_{73}P_{13}S_1$	626.909629	0.530	-/	013
		3				
629.055178	45.9	C ₁₁₆ H ₁₄₁ N ₄₂ O ₆₀ P ₁₁ S ₁	629.055795	0.980	-6	w11
		1				
629.585589	17.1	C ₃₈ H ₇₃ N ₆ O	629.585135	0.720	-2	
629.888011	6.7	C ₃₀ H ₂ NO ₁₀ P ₂ S	629.888014	0.000	-2	
632 404431	16.0	CoaHzaNooOoaPcSc	632 404566	0 210	-3	v6 - B(mC)
633 817008	12.8	$C_{1}H_{1}$	633 817108	-	_1	v8 - B(A)
000.017000	12.0	0811110011250421 707	000.017100	1 1 2 0	-4	, - (· ·)
60E 0E7046	07.0		625 050202	0.050	F	710 B(C)
035.057840	27.9	$C_{100}H_{118}N_{35}O_{50}P_9S_9$	035.058383	0.850	-5	CH3
635 251314	96	Coold to No O So	635 251341	0.040	-1	0.10
636 315657	8.0 8.2		636 316001	0.040	- 1 1	v8 - B(mC)
620.020004	0.2		620.02004	0.080		,0 2(0)
039.038094	∠J.U		039.03024	0.230	-1	
040.555532	1.8	$U_3HU_8P_4S_{11}$	040.555521	0.020	-8	L O
644.142043	112.3	$C_{24}H_{32}N_5O_{12}PS$	644.143303	1.956	-1	02
647.445705	12.7	$C_{39}H_{60}N_4O_2P$	647.445938	0.360	-1	
650.644193	21.0	$C_{101}H_{123}N_{28}O_{56}P_{10}S_1$	650.644969	1.190	-5	c10 - 6H, d10 -

657.431926	51.4	$\begin{array}{c} C_{166}H_{200}N_{51}O_{88}P_{15}S_{1}\\ {}_{5}\end{array}$	657.433269	2.040	-8	M - 8H - CH4 - A, M - 8H - CH4 - dA
657.747255 659.436168	247.9 180.3	$C_{66}H_{82}N_{16}O_{35}P_5S_5$	657.747887 650.437182	0.961	-3 8	b6 М - 8Н - А. М -
039.430100	109.5	5	039.437 102	1.540	-0	8H - dA
660.686436	10.4	C ₁₆₇ H ₂₀₂ N ₅₃ O ₈₇ P ₁₅ S ₁	660.68663	0.290	-8	M - 8H - mC, M - 8H - dC
665.570689	120.3	$C_{77}H_{128}N_{12}O_{55}P_{14}S_4$	665.570486	0.300	-4	
667.099483	244.0	$C_6H_{10}N_{34}OP_3$	667.099516	0.050	-2	
668.077100	8.3	$C_8H_{15}N_{25}O_7PS_2$	668.077081	0.030	-4	
669.147209	105.3	$C_{27}H_{36}N_4O_8P_3S$	669.14722	0.020	-1	
671.123176	6.5	$C_{30}H_{24}N_8O_7PS$	671.123177	0.000	-2	
671.873093	88.2	$C_{106}H_{128}N_{40}O_{52}P_9S_9$	671.875073	2.950	-5	y10
672.300599	10.5	$C_{24}H_{42}N_{13}O_8S$	672.30055	0.070	-1	
674.089461	1718. 4	$C_{66}H_{81}N_{23}O_{32}P_5S_5$	674.09087	2.090	-3	у6
674.754557	30.8	$C_{71}H_{207}N_{24}O_{12}P_{12}S_2$	674.754488	0.100	-1	
674.754914	125.9	$C_{71}H_{207}N_{24}O_{12}P_{12}S_2$	674.754488	0.630	-3	
676.316933	3240. 6	$\begin{array}{c} C_{172}H_{209}N_{56}O_{88}P_{15}S_{1}\\ {}_{5}\end{array}$	676.318994	3.050	-8	M - 8H
676.814953	323.4	$C_{10}H_{10}N_{10}O_6P_9S$	676.814956	0.000	-1	
677.654698	677.3	C ₁₀₆ H ₁₂₈ N ₃₃ O ₅₆ P ₁₀ S ₁ 0	677.655868	1.730	-5	d10 - H2O, c10 - 6H
679.112368	178.9	$C_7H_{21}N_{24}O_9P_2S$	679.112477	0.160	-1	
679.112403	1440. 4	$C_{46}H_{57}N_{16}O_{21}P_3S_3$	679.113508	1.630	-2	y4
683.724256	1004. 2	$C_{66}H_{81}N_{16}O_{36}P_6S_6$	683.725528	1.860	-3	d6 - H2O, c6 - 4H
685.057039	132.6	$C_{86}H_{104}N_{26}O_{46}P_8S_8$	685.057165	0.180	-4	d8 - H2O, c8 - 5H
687.063626	48.8	$C_{86}H_{104}N_{30}O_{43}P_8S_8$	687.064053	0.620	-4	x8 - 5H, w8 - H2O
687.260687	22.3	$C_{106}H_{126}N_{40}O_{53}P_{10}S_1$	687.260093	- 0.860	-5	x10 - 7H
689.051115	45.7	$C_{11}H_{25}N_{12}O_{15}P_4$	689.05183	1.040	-1	
689.077193	11.4	$C_{37}H_{23}O_{10}P_2$	689.077195	0.000	-1	
700.068793	233.2	$C_{66}H_{80}N_{23}O_{33}P_6S_6$	700.068511	-	-3	w6 - H2O, x6 -
				0.400		4H
701.397176	5.7	$C_{23}H_{49}N_{20}O_4S$	701.397185	0.010	-1	
703.517556	14.0	C ₄₃ H ₇₇ OP ₂ S	703.517586	0.040	-2	
706.069608	115.3	$C_9H_{25}N_{23}O_2P_5S_2$	706.069658	0.070	-1	
706.571653	26.7	$C_{46}H_{57}N_{12}O_{24}P_4S_4$	706.572648	1.410	-2	c4
709.565242	1469. 6	$C_{91}H_{110}N_{26}O_{48}P_8S_8$	709.56636	1.570	-4	b9 - B(A) - H2O, a9 - B(A)
716.070118	98.5	$C_{71}H_{86}N_{16}O_{38}P_6S_6$	716.068513	-	-3	a7 - 4H
716 101502	666.0		716 101151	2.240	2	27 - B(G)
/ 10.404000	000.2	U71H87N16U38P636	/ 10.404404	-	-3	ar - D(O)
710 000004	115 6		719 070060	0.180	2	w4 - H20 ×4 -
7 10.000094	115.0	$C_{46}\Pi_{56}\Pi_{16}O_{22}P_4O_4$	/ 10.0/ 9909	- 1 200	-2	3H
720 074873	18.0		720 074618	-	_4	v9 - B(A)
120.014010	10.0	0911111211300471 808	720.074010	0.350	-7	J - ()
722,573475	21.8	C01H110N22O46P0S0	722,573514	0.050	-4	y9 - B(mC)
726.000900	7.4	$C_{33}H_{23}N_{5}OP_{3}S_{4}$	726,00038	0.720	-1	- <i>•</i>
730.414408	7.2	$C_{38}H_{71}NO_{2}P_{3}S_{2}$	730.414457	0.070	-1	
731.374546	5.2	$C_{32}H_{64}N_2O_{10}PS_2$	731,374549	0.000	-3	
732.727678	7.1	$C_{136}H_{165}N_{46}O_{74}P_{13}S_{1}$	732,728432	1.030	-6	w13 - H2O, x13
735.879743	46.2	3 C116H141N42O50P40S4	735.879712	-	-5	- 7H y11
		0		0.040	-	-
739.412986	12.4	Č ₄₉ H ₅₁ N ₆ O	739.412984	0.000	-1	

741.978350 747.082836	15.8 185.8	$C_4H_{12}N_{31}P_8$	741.979839 747.082708	2.010	-1 -1	w2 - H2O. x2 -
	100.0			0.170	-1	2H
751.357716	23.8	C ₁₆₇ H ₂₀₄ N ₅₁ O ₈₇ P ₁₅ S ₁	751.357427	- 0.380	-7	M - 8H - dG, M - 8H - G
753.837454	606.0	C ₉₆ H ₁₁₇ N ₃₅ O ₄₇ P ₈ S ₈	753.838241	1.040	-4	у9
756.069827	5.6	$C_{143}H_{173}O_{74}N_{46}P_{13}S_1$	756.069657	-	-6	y14 - B(dA) -
		3		0.220	-	H2O, b14 - 8H, z14 - B(dA)
759.990140	5.9	C ₁₂ H ₁₄ N ₁₉ O ₁₃ S ₄	759.99068	0.710	-1	()
762.082244	296.4	$C_{18}H_{20}N_{17}O_{14}S_2$	762.082254	0.010	-1	
766.753748	12.4	$C_{76}H_{02}N_{21}O_{30}P_6S_6$	766.754257	0.660	-3	a7, b7 - H2O
767,996171	7.6	$C_{15}H_0N_{21}O_{12}P_2$	767,995789	0.500	-1	
772,756870	23.9	$C_{76}H_{04}N_{21}O_{40}P_6S_6$	772,757779	1.180	-3	b7
773 321818	9.0	C_{0} H ₄₄ N ₂ O ₄₀ P ₀ S ₀	773 321472	-	-4	w9 - H2O, x9 -
110.021010	0.0	096111610350481 909	110.021112	0 450	•	5H
778.578321	21.4	$C_{148}H_{178}O_{74}N_{51}P_{13}S_1$	778.578739	0.540	-6	z14, y14 - H2O
		3				. 7
780.764421	694.9	$C_{76}H_{94}N_{25}O_{38}P_6S_6$	/80./65268	1.080	-3	y/
781.429049	37.5	C ₂₃ H ₅₄ N ₂₂ O ₇ P	781.428893	0.200	-1	
782.097432	21.5	$C_{46}H_{28}NO_4P_4$	782.09743	0.000	-1	
787.089053	166.9	$C_{15}H_{28}N_{14}O_{18}PS_2$	787.089053	0.000	-1	
789.597782	14.5	$C_{44}H_{84}N_6P_3$	789.597581	0.250	-2	
791.477932	46.9	$C_{126}H_{152}N_{40}O_{65}P_{11}S_1$	791.477745	-	-5	b12 - H2O, a12
		1		0.240		
797.606186	6.7	$C_{16}H_6NO_7P_6S_9$	797.606188	0.000	-2	
798.734813	32.1	$C_{76}H_{93}N_{21}O_{41}P_7S_7$	798.73542	0.760	-3	d7 - H2O, c7 -
813 081499	12.6	$C_{rr}H_{ro}O_{r}P_{r}$	813 081492	0.010	-1	40
818 108344	388.6	CroHooN4000P4S4	818 108589	0.300	-2	b5 - H2O, a5
818 109338	135.7	$C_{0}H_{40}N_{00}O_{47}$	818 10944	0.000	_1	,
819 105046	20.7	$C_{r_0}H_{r_0}N_{r_0}O_{r_0}P_{r_0}S_{r_0}$	819 104509	-	-2	b5 - NH2
010.100010	20.1	0561 1681 130 291 404	010.101000	0 660	-	
827 113825	24 3	Carlon Na OssPasa	827 113871	0.000	-2	b5
831 414901	93.3	$C_{56}H_{70}N_{14}O_{29}H_{4}O_{4}$	831 414346	-	-2	a8 - B(G)
001.414001	00.0		001.414040	0 670	U	- (-)
831 734304	8.0	NacOvePaSe	831 73432	0.020	_1	
839 125676	198 5	$C_{23}O_{12}O_{2}O_{3}O_{3}P_{4}S_{4}$	839 125105	-	-2	v5
000.120070	100.0	05617014180271 404	000.120100	0.680	2	j -
860.286133	7.0	C126H165N46O60P12S1	860,286877	0.860	-5	z13, y13 - H2O
	-	2			-	
865.022312	44.7	$C_{23}H_{42}N_2O_{15}P_9$	865.022925	0.710	-1	
866.080752	16.3	$C_{56}H_{69}N_{14}O_{30}P_5S_5$	866.080333	-	-2	c5 - 3H, d5 -
				0.480		H2U
877.582481	17.3	C ₁₆ HN ₃ O ₁₃ P ₁₃ S	877.582463	0.020	-2	
878.078549	7.1	$C_{47}H_8N_{15}O_6$	878.078747	0.230	-2	
881.747870	9.4	$CH_{3}N_{27}O_{7}P_{7}S_{5}$	881.748114	0.280	-3	
881.763772	45.1	C ₈₆ H ₁₀₄ N ₂₆ O ₄₄ P ₇ S ₇	881.764149	0.430	-3	a8, b8 - H2O
887.097606	42.7	$C_{56}H_{71}N_{18}O_{29}P_5S_5$	887.096848	-	-2	w5
				0.850		
890.443697	7.1	C ₈₆ H ₁₀₆ N ₃₀ O ₄₂ P ₇ S ₇	890.443522	-	-3	у8
				0.200		
906.136910	11.3	$C_{13}H_{24}N_{35}O_5P_4S$	906.137632	0.800	-1	
915.148178	12.6	$C_{38}H_{39}N_6O_{13}S_4$	915.146344	2.000	-1	
941.052742	9.5	$C_{23}H_{45}N_6O_{16}P_8S$	941.05192	0.870	-1	
946.425379	22.0	$C_{91}H_{111}N_{26}O_{48}P_8S_8$	946.424239	-	-3	a9 - B(A), b9 -
				1.200		B(A) - H2O
953.105694	5.3	$C_{36}H_{61}O_3P_4S_9$	953.106308	0.640	-2	
966.059216	7.2	$C_{14}H_7N_{43}O_4P_3S$	966.060522	1.350	-1	
975.073500	5.5	$C_{18}H_{31}N_{20}O_{18}S_5$	975.073424	0.080	-1	
978.120325	29.6	$C_{66}H_{81}N_{16}O_{34}P_5S_5$	978.120186	-	-2	b6 - H2O, a6

				0.140		
984.069486 987.125702	32.2 7.3	C ₂₅ H ₅₃ N ₇ O ₁₀ P ₁₁ S C ₆₆ H ₈₃ N ₁₆ O ₃₅ P ₅ S ₅	984.069393 987.125469	0.090	-1 -2	b6
992.075975 993.081995 1000.57532	15.1 22.4 5.1	C ₁₆ H ₃₈ N ₁₉ O ₁₇ S ₇ C ₃₁ H ₅₁ N ₆ O ₉ P ₁₀ S C ₂₁ H ₇ N ₂ O ₁₅ P ₆ S ₉	992.074353 993.081992 1000.57640	0.240 1.640 0.000 1.080	-1 -1 -2	
5 1015.18928	16.8	$C_{36}H_{45}O_{17}N_{10}P_2S_2$	4 1015.18863	-	-1	b3
4 1022.16579	10.1	$C_{34}H_{64}N_7O_3P_{12}S$	1022.16482	0.640 0.950	-1	
9 1022.18529	71.2	$C_{36}H_{42}O_{15}N_{13}P_2S_2$	8 1022.18454 7	-	-1	y3 - H2O, z3
0 1026.09249	5.1	$C_{66}H_{82}N_{16}O_{36}P_6S_6$	7 1026.09193	0.730 - 0.550	-2	c6 - 3H, d6 - H2O
1034.08568	11.4	$C_{22}H_{46}N_{19}O_7P_6S_5$	1034.08623 6	0.530	-1	
4 1039.08960 0	8.2	$C_{27}H_{26}N_{30}O_3P_3S_4$	0 1039.09053 4	0.900	-1	
1040.19477 0	505.5	$C_{36}H_{44}O_{16}N_{13}P_2S_2$	1040.19511 2	0.330	-1	уЗ
1041.20124 7	49.1	$C_{18}H_{35}N_{28}O_{21}P_2$	- 1041.20122 8	0.020	-1	
1075.11107 8	62.5	$C_{71}H_{88}N_{16}O_{38}P_6S_6$	1075.11032	- 0 710	-2	b7 - B(G) - H2O, a7 - B(G)
1082.10703 7	26.7	$C_{33}H_{62}N_9O_2P_{14}S$	1082.10793 5	0.830	-1	
1091.09541 5	5.4	$C_{54}H_{30}N_{14}P_7$	1091.09467	0.680	-1	
1091.12022 8	16.1	$C_{32}H_{51}O_{33}S_4\\$	1091.12009 2	0.120	-1	
1102.15427 3	6.5	$C_{24}H_{70}N_{15}O_2P_{10}S_6$	_ 1102.15428 7	0.010	-1	
1107.11379 9	19.9	$C_{30}H_7N_{46}S_3$	1107.11294 2	0.770	-1	
1118.12884 2	22.3	$C_{36}H_{43}O_{17}N_{13}P_3S_3$		- 0 720	-1	w3 - H2O, x3 - 2H
	28.1	$C_{36}H_{45}O_{18}N_{13}P_3S_3$	1136.1386	- 2 377	-1	w3
1150.63800 5	11.1	$C_{76}H_{93}N_{21}O_{39}P_6S_6$	1150.63502 4	- 2 590	-2	b7 - H2O, a7
1169.05029	9.8	$C_{80}H_{23}N_2P_2S_3$	1169.05041	0.100	-1	
1171.65154 7	10.6	$C_{76}H_{95}N_{25}O_{38}P_6S_6$	1171.65154	- 0.010	-2	у7
, 1178.05239 o	12.9	$C_{79}H_{27}NP_3S_3$	1178.05239 8	0.000	-1	
1208.15163	6.6	$C_{40}H_{49}N_{11}O_{21}P_3S_3$	1208.14849 7	- 2 600	-1	y4 - B(dA) - CH4
1225.17501	10.2	$C_{87}H_{31}N_4P_2S$, 1225.17501 6	0.000	-1	
3 1234.16352 7	5.4	C ₈₆ H ₂₉ NO ₈ P	1234.16362 7	0.080	-1	
, 1247.62916 2	10.4	$C_{82}H_{92}N_2O_3PS_2$	/ 1247.62924 8	0.070	-2	
1317.20130 1	55.7	$C_{46}H_{56}N_{12}O_{22}P_3S_3$	1317.20126 1 Abs mean error	- 0.030 1.879	-1	b4 - H2O, a4

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Table S7 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ danvatirsen by IRMPD MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured	S/N	Elemental Composition	Theoretical	Error (ppm	Charg	Assignmen t	
1112		Composition	1112)	C	t	
319.015936	326. 8	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	- 0.060	-1	a5(T)w12, a4(T)w13, b4(T)x13, c4(T)y13, d4(T)z13, w4b13 - NH2, z5(T)d12, b5(T)x12, x5(T)b12, y5(T)c12, d6(T)z11, c5(T)y12, w7(T)a10, d5(T)z12, a6(T)w11, b6(T)x11, y7(T)c10, z7(T)d10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a12, w7(T)a10, w5(T)a10, w5(T)a12, w7(T)a10, w5(J1
344.022388	80.3	$C_{10}H_{12}N_5O_5PS$	344.022400	0.040	-1	b9(A)w8, w6(G)a11, d8(G)29, c8(G)y9, b8(G)x9, a8(G)w9, c7(G)y10, b7(G)x10, d7(G)z10, a7(G)w10, x6(G)b11, y8(A)d9, y6(G)c11, z6(G)d11, w8b9 - 1H	J2
360.042454	57.4	$C_{12}H_{15}O_6N_3PS$	360.042467	0.040	-1	x1 - 2H, c1 - 2H, d1 - H2O, w1 - H2O	J3
361.026462	103. 0	$C_{12}H_{14}O_7N_2PS$	361.026482	0.060	-1	w1 - NH3, d1 - NH3	
369.539723	146. 9	$C_{24}H_{31}O_{14}N_5P_2S_2$	369.539757	0.090	-2	d2	
378.041314	42.8	$C_{36}H_{43}O_{18}N_{13}P_3S_3$	378.041349	0.090	-3	w3	
378.053018 386.032911	56.8 54.4	C ₁₂ H ₁₇ O ₇ N ₃ PS C ₁₂ H ₁₄ N ₅ O ₆ PS	378.053032 386.032965	0.040 0.140	-1 -1	d1, w1 b3(dA)w14, z2(dG)d15, y2(dG)c15, x2(dG)b15, w3b14 - 1H, w2(dG)a15, y3(dA)d14, d3(dA)v14	J5
386.032911	54.4	$C_{11}H_{19}NO_8P_3$	386.032901	0.030	-1		
388.048703	15.6	$C_{12}H_{15}N_5O_6PS$	388.048615	0.230	-1		
398.982222 414.959383	48.1 192. 4	C ₁₀ H ₁₃ N ₂ O ₉ P ₂ S C ₁₀ H ₁₄ N ₂ O ₈ P ₂ S ₂	398.982249 414.959405	0.070 0.050	-1 -1	c6(T)w11, d4(T)x13, d6(T)x11, c4(T)w13, w7(T)c10, c5(T)w12, d5(T)x12,	J6

						$w_{5(T)c12}$	
414.959383	192.	$C_{10}H_{13}N_2O_8P_2S_2$	414.959405	0.050	-1	W3(1)012	
414.959455	4 79.7	$C_{10}H_{14}N_2O_8P_2S_2$	414.959405	- 0.120	-1	c6(T)w11, d4(T)x13, d6(T)x11, c4(T)w13, w7(T)c10, c5(T)w12, d5(T)x12, w5(T)x12, w5(T)c12	J7
417.052741 421.955313	47.6 9.9	$\begin{array}{l} C_{15}H_{18}N_2O_8PS\\ C_{10}H_{11}N_5O_6P_2S_2 \end{array}$	417.052697 421.955323	0.110 0.020	-1 -1	w5(1)c12 d8(G)x9 - H2O, x6(G)c11 - 1H, c8(G)w9 - H2O, w8(A)d9 - H2O, c8(G)x9 - 2H, d7(G)x10 - H2O, w8c9 - 2H, w6(G)c11 - H2O, x8(A)d9 - 1H, c7(G)x10 - 2H, c7(G)w10 -	3U
423.988698 431.693867	29.9 41.3	C ₉ H ₁₈ NO ₁₀ P ₄ C ₄₁ H ₄₇ N ₁₂ O ₂₁ P ₄ S ₄	423.988667 431.694284	0.070 0.970	-1 -3	H2O x4 - B(mC) -	
432.028283 439.965857	20.2 72.8	$\begin{array}{l} C_{79}H_{18}N_{11}O_7S_2\\ C_{10}H_{13}N_5O_7P_2S_2 \end{array}$	432.028285 439.965888	0.010 0.070	-3 -1	NH2 d8(G)x9, w6(G)c11, c7(G)w10, w8(A)d9, d7(G)x10,	J9
439.965857 442.059196 450 004372	72.8 63.4 11 1	C ₁₃ H ₂₂ NP ₈ C ₁₄ H ₂₃ NO ₉ P ₃ C ₁₂ H ₄₄ N₅O ₈ P ₂ S	439.965869 442.059116 450 004381	0.030 0.180 0.020	-1 -1 -1	c8(G)w9	
458.079170	15.2	$C_{17}H_{21}O_8N_3PS$	458.079247	0.170	-1	z2 - B(dG) - OC2H2, a2 - B(dU) - OC2H2	J1 0
465.981472	26.4	$C_{11}H_{20}NO_9P_4S$	465.981474	0.000	-1		
465.981472	26.4	$C_{12}H_{15}N_5O_7P_2S_2$	465.981538	0.140	-1	d3(dA)x14, w3c14, c3(dA)w14	J1 1
484.387795	18.7	$C_{46}H_{57}N_{16}O_{23}P_4S_4$	484.387742	- 0.110	-3	w4	
487.244768	11.1	$C_{76}H_{93}N_{25}O_{40}P_7S_7$	487.244948	0.370	-5	w7	
494.985578	98.3	$C_{12}H_{11}N_{12}OP_4S$	494.985546	0.060	-1		
504.014912	22.3	C ₁₇ H ₃₀ NS ₈	504.014943	0.060	-1		
507.090706	17.8	$C_{36}H_{44}O_{17}N_{10}P_2S_2$	507.090677	-	-2	b3	
_ /			- / / /	0.060			
512.996156	173. 0	$C_{16}H_{22}O_9P_5$	512.995741	0.810	-1		
519.593954	21.5	$C_{36}H_{43}O_{16}N_{13}P_2S_2$	519.593918	- 0.070	-2	уЗ	
519.992079	47.1	C ₁₈ H ₂₆ NOP ₈	519.992084	0.010	-1		
538.002646	166. 9	$C_{16}H_{21}N_3O_8P_5$	538.002223	0.790	-1		
540.549121	38.0	$O_2P_3S_{13}$	540.548589	0.990	-2		
553.052098	14.6	C ₈₆ H ₁₀₅ N ₃₀ O ₄₄ P ₈ S ₈	553.051900	- 0.360	-5	w8	
558.560494	7.4	$C_{36}H_{42}O_{17}N_{13}P_3S_3$	558.560380	- 0,200	-2	x3 - 3H, w3 - H2O	
561,106223	15.4	C₂₄H₃₀N₄O₂P₌	561,106235	0.020	-1		
567,565807	8.1	$C_{36}H_{44}O_{40}N_{42}P_{2}S_{2}$	567,565662	-	-2	w3	
201.000001	0.1		201.000002	0 260	-		
570,056437	81 7	$C_{20}H_4N_{42}O_2$	570,056555	0.210	-2		
010.000401	01.7		31 0.000000	0.210	-		

586.112617	53.0	$C_{19}H_{31}N_3O_{12}P_3$	586.112608	0.020	-1	
586.112701	21.6	$C_{23}H_{34}N_5OP_2S_4$	586.112693	0.010	-1	17 100 .7
598.799952	38.6	$C_{76}H_{92}N_{21}O_{41}P_7S_7$	598.799746	-	-4	d7 - H2O, c7 - 5H
600 070947	22.0		600 070706	0.340	2	
600.072047	33.U 35.2	$C_{32}\Pi_{11}N_9O_3P$	600.072790	0.090	-2 1	w7
009.300293	JJ.Z	C76F 194T 25 C 40F 7 C7	009.300004	- 0.470	-4	
618 537086	76		618 536953	0.470	-4	
639 039020	70.6		639 039014	0.220	- -	
644 143261	111	$C_{16}H_{24}N_{12}O_{4} = 0.5$ $C_{24}H_{24}O_{42}N_{5}PS$	644 143303	0.070	-1	b2
• • • • • • • • • • • • • • • • • • • •	3	- 24. 31 - 12. 3			-	
645.127354	15.8	$C_{28}H_{34}N_4O_4P_5$	645.127364	0.020	-1	
653.047679	7.3	C ₇₉ H ₉₆ N ₂₈ O ₄₂ P ₈ S ₈	653.048137	0.700	-4	w8 - B(T) -
656 070612	11 2		656 070256		1	C2H4 78 - C2H4
050.070015	11.5	C84H99N30C41F7S7	050.070550	- 0 300	-4	20 - 02114
657 748183	53 5		657 747887	0.590 -	-3	b6
001.140100	00.0	0661 1821 16 0 351 505	001.141001	0 450	-0	
658.079247	9.3	C11H15N23O6P3	658.079400	0.230	-3	
658.097320	50.1	$C_{46}H_{55}N_{12}O_{22}P_3S_3$	658.096992	-	-2	b4 - H2O, a4
				0.500		
659.684766	10.0	$C_5H_5N_9O_2P_{11}S_3$	659.684765	0.000	-2	
661.868677	7.3	$C_{106}H_{128}N_{33}O_{55}P_9S_9$	661.867718	-	-5	b10 - 6H
				1.450		
664.045544	89.8	$C_{23}H_{34}N_3O_4P_8$	664.045576	0.050	-2	
665.214662	30.4	$C_{25}H_{47}N_6O_3P_6$	665.214085	0.870	-1	h.4
667.102431	29.9	$C_{46}H_{57}N_{12}O_{23}P_3S_3$	667.102274	-	-2	D4
667 590904	15.0		667 500000	0.240	1	v8
007.000024 668.551347	10.2	$C_{86}\Pi_{105}\Pi_{30}U_{42}P_7S_7$	668 551330	0.000	-4 1	yo
669 149799	21.5		669 149786	0.020	-1	v2
000.140700	21.0	02411300111481 0	000.140700	0 020	-1	<u> </u>
670.026527	25.8	C11H13N23O3P5	670.026530	0.000	-3	
670.108240	28.0	$C_{46}H_{55}N_{16}O_{20}P_3S_3$	670.108225	-	-2	y4 - H2O, z4
				0.020		
674.091205	62.4	$C_{66}H_{81}N_{23}O_{32}P_5S_5$	674.090870	-	-3	y6
				0.500		
674.422158	14.4	$C_{22}H_{66}N_{11}O_4P_2S_2$	674.422140	0.030	-3	
676.193679	371.	$C_{172}H_{208}N_{56}O_{88}P_{15}S_1$	676.193016	-	-8	M - 9H
077 05 4000	6	5 0 11 N 0 D 0	077 050074	0.980	-	
677.854638	6.6	$C_{106}H_{127}N_{32}O_{57}P_{10}S_1$	677.852671	-	-5	010 - NH3
670 112559	57.0		670 112509	2.900	2	vA
079.115556	57.Z	C46H57N16O21F3O3	079.115506	-	-2	ут
680 111376	65	$C_{70}H_{10}N_0O_{17}S_0$	680 111390	0.070	-2	
683.725850	34.3	$C_{66}H_{81}N_{16}O_{36}P_6S_6$	683.725528	-	-3	d6 - H2O, c6 -
	••			0.470	C C	4H
684.390895	7.8	$C_{66}H_{81}N_{15}O_{37}P_6S_6$	684.389475	-	-3	d6 - NH2
				2.080		
685.056832	11.8	$C_{86}H_{104}N_{26}O_{46}P_8S_8$	685.057165	0.490	-4	d8 - H2O, c8 -
600 061253	115		600 061245	0.010	1	5H
700 068444	83	$C_{22} \Gamma_{26} \Gamma_{7} O_{11} \Gamma_{2} O_{2}$	700 068511	0.010	-1	w6 - H2O x6 -
700.000444	0.5		700.000311	0.100	-0	4H
706.068897	10.7	$C_{46}H_{56}N_{12}O_{24}P_4S_4$	706.068736	-	-2	d4 - H2O, c4 -
				0.230		ა⊓ სი ნ(1)
709.566719	59.4	$C_{91}H_{110}N_{26}O_{48}P_8S_8$	709.566360	-	-4	ру - В(А) - Н2О, а9 - В(А)
700 04 4050	10.0		700 040004	0.510	4	$h_{0} = B(\Lambda) N \sqcup 2$
709.814353	19.3	U91H109N25U49P8S8	109.812364	- 2 200	-4	ыз - D(A) - NПО
716 404357	44 6		716 404454	2.000 0.1/0	-3	a7 - B(G)
110.404007	4 +.0	U711 1871 N16U38F6U6	110.404404	0.140	-0	

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718.079869	8.7	$C_{46}H_{56}N_{16}O_{22}P_4S_4$	718.079969	0.140	-2	w4 - H2O, x4 -
722.076223	11.3	$C_{24}H_{30}O_{13}N_5P_2S_2$	722.076226	0.000	-1	зн d2 - H2O, c2 - 2H
726 001493	18.2		726 001499	0 010	-1	
732 071754	12/	C_{4} H_{2} O_{4} N_{2} P_{2} S_{2}	732 071800	0.080	_1	x2 - NH2
707.075740	14.0		707.075754	0.000	-1	
/3/.0/5/46	14.2	$C_{21}H_{31}N_{10}O_8P_6$	737.075754	0.010	-1	10
740.086792	8.4	$C_{24}H_{32}O_{14}N_5P_2S_2$	740.086791	0.000	-1	d2
747.083103	40.1	$C_{24}H_{29}O_{12}N_8P_2S_2$	747.082708	-	-1	w2 - H2O, x2 -
				0.530		2H
753 587785	10.2		753 586285	-	-4	v9 - 5H
100.001100	10.2	090.1110.033047.808	.00.000200	1 000	•	2
700 705004	24.0		700 765060	1.550	2	ν7
100.100034	34.0	$C_{76}\Pi_{94}\Pi_{25}O_{38}\Pi_{6}O_{6}O_{6}O_{6}O_{6}O_{6}O_{6}O_{6}O$	100.105200	-	-3	ÿï
				0.470		
818.108671	21.5	C ₅₆ H ₆₈ N ₁₄ O ₂₈ P ₄ S ₄	818.108589	-	-2	b5 - H2O, a5
				0.100		
827.113486	5.7	$C_{56}H_{70}N_{14}O_{20}P_4S_4$	827.113871	0.470	-2	b5
831 414376	20.8	Co. HooNo. OusP-S-	831 414346	_	_3	a8 - B(G)
001.414070	20.0		001.414040	0.040	-0	
000 404004	00.0		000 405405	0.040	~	. E
839.124994	32.0	$C_{56}H_{70}N_{18}O_{27}P_4S_4$	839.125105	0.130	-2	y5
840.015255	53.8	$C_{27}H_{44}NO_7P_6S_5$	840.015254	0.000	-1	
840.128425	17.9	C ₈₆ H ₁₉₉ N ₃ O ₄ P ₁₀ S	840.128425	0.000	-2	
887.097144	14.2	C ₅₆ H ₇₁ N ₁₈ O ₂₉ P ₅ S ₅	887.096848	-	-2	w5
		- 30 11 10 - 23 3 3		0.330		
999 125/69	65		999 125/60	0.000	1	
000.120400	0.5	$C_{67}I_{14}I_{15}$	000.120409	0.000	-1	
906.135901	8.6	$C_{15}H_{42}N_{17}O_{16}P_2S_4$	906.135901	0.000	-1	
941.051857	18.8	$C_{22}H_{51}N_2O_{18}P_{10}$	941.051856	0.000	-1	
947.139794	28.3	C ₄₂ H ₂₇ N ₈ O ₁₉	947.139794	0.000	-1	
947.139937	11.2	C15H44N22O10PS7	947.139885	0.050	-1	
956,151449	28.0	C25HenNOnP2Se	956,151449	0.000	-1	
956 151596	10.6	CuoHu-N-Oo-PS	956 151540	0.060	_1	
070 100270	14.0		070 1001040	0.000	- I	b6 - H2O - a6
976.120379	14.2	$C_{66}\Pi_{81}\Pi_{16}O_{34}P_5O_5$	970.120100	-	-2	50 - 1120, 80
				0.200		
984.068731	32.2	$C_{15}H_{45}N_{23}O_2P_{11}S_2$	984.068731	0.000	-1	
984.068849	11.8	$C_{12}H_{32}N_{19}O_{26}P_2S_2$	984.068802	0.050	-1	
993.080976	7.5	C ₂₉ H ₃₃ N ₁₄ O ₁₆ S ₅	993.080800	0.180	-1	
1015.18856	8.4	$C_{36}H_{45}O_{17}N_{10}P_2S_2$	1015.18863	0.060	-1	b3
8	-	- 00 +0 - 11 10 2 2	0			
1022 183/1	13.6	Carlly OveN v PaSa	1022 18454	1 1 1 0	_1	v3 - H2O <i>7</i> 3
2	15.0	C361 142 C151 N13F 2C2	7	1.110	- 1	<i>yo</i> 1120, 20
3	40.0		1	0.440		
1034.08454	12.9	$C_{19}H_{44}N_{15}O_{19}P_8$	1034.08443	0.110	-1	
9			4			
1040.19545	106.	C ₃₆ H ₄₄ O ₁₆ N ₁₃ P ₂ S ₂	1040.19511	-	-1	y3
1	0		2	0.330		
1075.11090	20.1	C71H88N16O38P6S6	1075.11032	-	-2	b7 - B(G) -
1			0	0 540	_	H2O, a7 - B(G)
1001 11721	70		1001 11755	0.040	1	
1091.11731	7.9	C35H37N24OF6S3	1091.11755	0.220	- 1	
0			1			
1102.15001	5.8	$C_{25}H_{64}N_5O_{24}P_4S_5$	1102.1500 <i>1</i>	0.060	-1	
0			5			
1107.11224	6.5	$C_{26}H_{65}N_{14}O_2P_{10}S_6$	1107.11208	0.140	-1	
2			8			
1118 12864	96	$C_{22}H_{22}O_{47}N_{42}P_{2}S_{2}$	1118 12803	-	-1	w3 - H2O. x3 -
5	0.0		6	0 540		2H
1400 40750	24.0		1100 10000	0.040	4	w3
1136.13758	31.2	$C_{36}H_{45}O_{18}N_{13}P_3S_3$	1136.13860	0.900	-1	w5
2			0			
1141.12045	37.2	C ₇₉ H ₁₇ N ₈ O ₂ S	1141.12006	0.340	-1	
9			7			
1201.15269	7.3	C ₈₇ H ₃₁ O ₂ P ₂ S	1201.15254	0.120	-1	
6	-		9			
1317 20130	59 1		1317 20126	_	_1	b4 - H2O. a4
1011.20100	00.1	-40 100 12 22 303	1011.20120			- /

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2	1	0.030
	Abs mean	0.407
	error	
	Abs mean	0.582
	std dev	

Table S8 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ danvatirsen by UVPD MS/MS, internal fragments marked by character (J), base losses are shown inside the parenthesis.

Measured mz	S/N	Elemental Composition	Theoretical <i>mz</i>	Error (ppm	Charg e	Assignmen t	
405 0 4050 4	0.40.4		405 0 40 4 40)		-	
165.949534 317.024069	243.1 45.9	CH ₃ N ₃ OP ₃ C ₁₀ H ₁₃ N ₃ O ₅ PS	165.949446 317.024077	0.530 0.020	-1 -1	w4(mC)a13 - 1H, w4b13 - H2O, z4(mC)d13 - 1H, x4(mC)b13 - 1H, y4(mC)c13 - 1H	J1
319.015954	290.6	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	- 0.110	-1	a5(T)w12, a4(T)w13, b4(T)x13, c4(T)y13, d4(T)z13, w4b13 - NH2, z5(T)d12, b5(T)x12, x5(T)b12, y5(T)c12, d6(T)z11, c5(T)y12, w7(T)a10, d5(T)z12, a6(T)w11, b6(T)x11, y7(T)c10, z7(T)d10, w5(T)a12, x7(T)b10	J2
328.027552	46.2	$C_{10}H_{12}N_5O_4PS$	328.027486	- 0.200	-1	x7(1)b10 z6(G)c11, y8(A)c9, c8(G)z9, a8(G)x9, c7(G)z10, a7(G)x10, a9(A)w8, x8(A)b9, w8(A)a9, b9(A)x8, z8(A)d9	J3
343.014588 360.042496	303.8 44.3	$C_{10}H_{11}N_5O_5PS$ $C_{12}H_{15}O_6N_3PS$	343.014575 360.042467	- 0.040	-1	w6b11 - H2O, d7(G)z10 - 1H, c7(G)y10 - 1H, z6(G)d11 - 1H, b7(G)x10 - 1H, a7(G)w10 - 1H, d8(G)z9 - 1H, x6(G)b11 - 1H, w6(G)c11 - 1H, w8b9 - 2H, y8(A)d9 - 1H, w6(G)a11 - 1H, a8(G)w9 - 1H, b9(A)w8 - 1H, b8(G)x9 - 1H, c8(G)y9 - 1H x1 - 2H, c1 -	J4
361.026562	68.3	$C_{12}H_{14}O_7N_2PS$	361.026482	0.080 -	-1	2H, d1 - H2O, w1 - H2O w1 - NH3, d1 -	
070 000400	05.4		070 000050	0.220	-	NH3	16
370.038128	95.1	$C_{12}H_{14}N_5O_5PS$	370.038050	- 0.210	-1	c3(dA)y14, a3(dA)w14,	JØ

						w3(dA)a14, y3(dA)c14, z2(dG)c15, b3(dA)x14, z3(dA)d14, x3(dA)b14, d3(dA)z14	
378.053085	105.8	$C_{12}H_{17}O_7N_3PS$	378.053032	- 0.140	-1	d1, w1	
386.032973	114.9	$C_{12}H_{14}N_5O_6PS$	386.032965	0.020	-1	b3(dA)w14, z2(dG)d15, y2(dG)c15, x2(dG)b15, w3b14 - 1H, w2(dG)a15, y3(dA)d14, d3(dA)y14	J7
398.982326	98.2	$C_8H_{16}O_{12}PS_2$	398.982629	0.760	-1	-C(T):::11	10
414.959499	83.3	C ₁₀ H ₁₄ N ₂ O ₈ P ₂ S ₂	414.959405	- 0.230	-1	co(1)w11, d4(T)x13, d6(T)x11, c4(T)w13, w7(T)c10, c5(T)w12, d5(T)x12, w5(T)c12	Jo
423.988720	160.6	C ₉ H ₁₈ NO ₁₀ P ₄	423.988667	0.130	-1		10
439.965913	118.1	C ₁₀ H ₁₃ N ₅ O ₇ P ₂ S ₂	439.965888	- 0.060	-1	08(G)x9, w6(G)c11, c7(G)w10, w8(A)d9, d7(G)x10, c8(G)w9	79
450.004400	171.2	C ₁₁ H ₂₀ NO ₁₀ P ₄	450.004317	0.190	-1		
450.004488	70.5 107.2	$C_{11}H_{20}NO_{10}P_4$	450.004317	0.380	-1 1	d3(dA)x14	.11
405.901595	107.5	C ₁₂ I I ₁₅ IN ₅ O ₇ F ₂ S ₂	403.901330	- 0.120	-1	w3c14, c3(dA)w14	0
481.976495	78.0	$C_{12}H_{15}N_5O_8P_2S_2$	481.976452	- 0.090	-1	d3w14, w2(dG)c15, w3(dA)d14	J1 1
484.387651	47.9	$C_{46}H_{57}N_{16}O_{23}P_4S_4$	484.387742	0.190	-3	w4`´´	
512.996331	115.6	$C_{17}H_{26}O_4P_5S_2$	512.996610	0.540	-1	43 31	
554.558523	156.9	$C_{36}H_{44}O_{19}N_{10}P_3S_3$	554.558508	- 0.030	-2	u3 - 3H	
566.557816	60.3	C ₃₆ H ₄₂ O ₁₈ N ₁₃ P ₃ S ₃	566.557837	0.040	-2	w3 - 4H	
567.565906	42.0	$C_{36}H_{44}O_{18}N_{13}P_3S_3$	567.565662	-	-2	w3	
501 062400	33.0		501 062140	0.430	3	w5	
391.002499	33.0	05611701 1 8029 F 505	591.002140	- 0.610	-3	wo	
595.075718	53.1	$C_{41}H_{49}N_{10}O_{20}P_3S_3$	595.075528	- 0.320	-2	y4 - B(dG) - NH3, b4 - B(T) - H2O, a4 -	
603.302333	5.4	C76H94N21O42P7S7	603.302387	0.090	-4	d7	
609.308403	104.9	C ₇₆ H ₉₄ N ₂₅ O ₄₀ P ₇ S ₇	609.308004	-	-4	w7	
000 000005	50.0		620 020274	0.650	4		
639.039335 644 143460	59.3 66 5	$C_{25}H_{20}O_{18}P$ $C_{25}H_{20}O_{18}P$	639.039274	0.100	-1 -1	b2	
544.140400	00.0	C241 131 C121 151 C	577.170000	0.240			
651.744552	8.1	$C_9H_{15}NO_7P_{13}$	651.744306	0.380	-1		
651.744755	48.8	$C_{66}H_{80}N_{16}O_{34}P_5S_5$	651.744365	- 0.600	-3	b6 - H2O, a6	
657.593238	234.3	$C_{46}H_{54}N_{12}O_{22}P_3S_3$	657.593080	- 0 240	-2	a4 - 3H	
658.097591	90.1	$C_{46}H_{55}N_{12}O_{22}P_3S_3$	658.096992	0.240 - 0.910	-2	b4 - H2O, a4	
659.311877	43.4	$C_{167}H_{203}N_{51}O_{88}P_{15}S_1$	659.311204	-	-8	M - 9H - A, M -	

		5		1.020		9H - dA
664.045786 674.091273	113.5 9.1	$\begin{array}{l} C_{15}H_{18}N_7O_{23}\\ C_{66}H_{81}N_{23}O_{32}P_5S_5 \end{array}$	664.045953 674.090870	0.250	-1 -3	у6
676.068145	888.2	$C_{172}H_{207}N_{56}O_{88}P_{15}S_1$	676.067037	0.600 -	-8	M - 10H
679.113654	27.1	$^{5}C_{46}H_{57}N_{16}O_{21}P_{3}S_{3}$	679.113508	1.040 - 0.220	-2	y4
682.226086	28.9	$C_{126}H_{153}N_{44}O_{66}P_{12}S_1$	682.225023	- 1 560	-6	w12 - 7H
689.560130	25.1	$C_{86}H_{106}N_{26}O_{47}P_8S_8$	689.559806	- 0.470	-4	d8
691.064015	18.8	$C_{106}H_{129}N_{40}O_{54}P_{10}S_1$	691.063771	- 0.350	-5	w10
691.567183	38.9	C ₈₆ H ₁₀₆ N ₃₀ O ₄₄ P ₈ S ₈	691.566694	- 0.710	-4	w8
705.399926 706.072882	18.8 22.6	$\begin{array}{l} C_{66}H_{80}N_{23}O_{34}P_6S_6\\ C_{66}H_{82}N_{23}O_{34}P_6S_6 \end{array}$	705.400149 706.072032	0.320 - 1 200	-3 -3	w6 - 5H w6
709.566728	16.5	$C_{91}H_{110}N_{26}O_{48}P_8S_8$	709.566360	- 0.520	-4	b9 - B(A) - H2O, a9 - B(A)
716.405055	13.7	$C_{71}H_{87}N_{16}O_{38}P_6S_6$	716.404454	- 0.840	-3	a7 - B(G)
722.076174	75.3	$C_{24}H_{30}O_{13}N_5P_2S_2$	722.076226	0.070	-1	d2 - H2O, c2 - 2H
727.085530	70.0	$C_{46}H_{58}N_{16}O_{23}P_4S_4$	727.085251	- 0.380	-2	w4
732.072024	14.8	$C_{24}H_{28}O_{12}N_7P_2S_2$	732.071809	- 0.290	-1	x2 - NH2
735.207237	9.7	C ₁₆₀ H ₁₉₅ O ₈₄ N ₅₃ P ₁₅ S ₁ 5	735.207567	0.450	-7	w15, d15
740.086718 743.079448	36.5 94.2	C ₂₄ H ₃₂ O ₁₄ N ₅ P ₂ S ₂ C ₉₆ H ₁₁₄ N ₃₁ O ₄₈ P ₈ S ₈	740.086791 743.078027	0.100 - 1.910	-1 -4	d2 a9 - 5H
747.082583	62.3	$C_{24}H_{29}O_{12}N_8P_2S_2$	747.082708	0.170	-1	w2 - H2O, x2 - 2H
749.084961	17.4	$C_{96}H_{114}N_{35}O_{46}P_8S_8$	749.083644	- 1.760	-4	z9 - 5H
750.063031	7.0	$C_{116}H_{141}N_{38}O_{62}P_{11}S_1$	750.062351	- 0.910	-5	d11 - 6H
751.500569	11.1	$C_{167}H_{205}N_{51}O_{87}P_{15}S_1$	751.501402	1.110	-7	M - 7H - G, M - 7H - dG
753.786050	15.1	$C_{167}H_{205}N_{51}O_{88}P_{15}S_1$	753.786390	0.450	-7	M - 7H - dA, M - 7H - A
753.838417	5.3	C ₉₆ H ₁₁₇ N ₃₅ O ₄₇ P ₈ S ₈	753.838241	- 0.230	-4	у9
754.867520	9.0	$C_{116}H_{141}N_{42}O_{60}P_{11}S_{1}$	754.866845	- 0.890	-5	w11 - 6H
765.093245 766.754841	164.7 143.0	$C_{24}H_{31}O_{13}N_8P_2S_2$ $C_{76}H_{92}N_{21}O_{39}P_6S_6$	765.093273 766.754257	0.040	-1 -3	w2 a7, b7 - H2O
772.792573	211.2	$C_{172}H_{208}N_{56}O_{88}P_{15}S_1$	772.791939	- 0.820	-7	M - 9H
774.762409	16.0	${\overset{_{5}}{C}}_{76}{H}_{92}{N}_{25}{O}_{37}{P}_{6}{S}_{6}$	774.761746	- 0.860	-3	y7 - H2O, z7
777.573549	35.6	$C_{96}H_{117}N_{35}O_{49}P_9S_9$	777.572157	- 1 700	-4	w9 - 5H
780.765759	15.7	$C_{76}H_{94}N_{25}O_{38}P_6S_6$	780.765268	- 0 620	-3	у7
791.277281	129.4	$C_{126}H_{151}N_{40}O_{65}P_{11}S_1$	791.276180	- 1.390	-5	a12 - 6H

796.282183	8.8	$C_{126}H_{152}N_{44}O_{63}P_{11}S_1$	796.282238	0.070	-5	y12 - H2O, z12
804.739567	15.7	$^{1}C_{76}H_{95}N_{21}O_{42}P_{7}S_{7}$	804.738941	- 0 780	-3	d7
812.747049	67.8	$C_{76}H_{95}N_{25}O_{40}P_7S_7$	812.746430	- 0 760	-3	w7
818.108812	85.4	$C_{56}H_{68}N_{14}O_{28}P_4S_4$	818.108589	-	-2	b5 - H2O, a5
819.072842	210.4	$C_{126}H_{155}N_{44}O_{66}P_{12}S_1$	819.073048	0.270	-5	w12
823.085229	40.3	² C ₁₀₆ H ₁₂₇ N ₃₃ O ₅₄ P ₉ S ₉	823.083826	- 1 700	-4	a10 - 5H
830.120351	70.1	$C_{56}H_{68}N_{18}O_{26}P_4S_4$	830.119822	-	-2	y5 - H2O, z5
831.414997	15.4	$C_{81}H_{99}N_{21}O_{43}P_7S_7$	831.414346	- 0 780	-3	a8 - B(G)
833.276084	7.7	$C_{131}H_{160}N_{41}O_{69}P_{12}S_1$	833.275978	- 0.130	-5	y13 - B(A) - H2O, z13 -
835.593335	9.9	C ₁₀₆ H ₁₂₇ N ₄₀ O ₅₁ P ₉ S ₉	835.593020	-	-4	B(A), b13 - 7H z10, y10 - H2O
839.125443	12.8	$C_{56}H_{70}N_{18}O_{27}P_4S_4$	839.125105	-	-2	у5
840.095798	42.7	$C_{106}H_{129}N_{40}O_{52}P_9S_9$	840.095661	0.400 - 0.160	-4	y10
851.824789	24.3	$C_{106}H_{131}N_{33}O_{57}P_{10}S_1$	851.824295	- 0.580	-4	d10
855.084729	13.2	${\overset{_{0}}{C}}{}_{136}H_{165}N_{43}O_{70}P_{12}S_{1}$	855.084015	-	-5	a13 - 6H
860.286768	230.1	$^{2}C_{136}H_{165}N_{46}O_{69}P_{12}S_{1}$	860.286877	0.830	-5	z13, y13 - H2O
863.578875	16.5	$C_{106}^{2}H_{128}N_{40}O_{54}P_{10}S_{1}$	863.577620	- 1 450	-4	w10 - 6H
866.080330	5.2	$^{0}C_{56}H_{69}N_{14}O_{30}P_{5}S_{5}$	866.080333	0.000	-2	c5 - 3H, d5 - H2O
870.103012	11.9	$C_{31}H_{34}O_{15}N_7P_2S_2$	870.103503	0.560	-1	z3 - B(dA) -
871.328786	6.4	$C_{111}H_{133}N_{33}O_{58}P_{10}S_1$	871.326936	- 2 120	-4	a11 - 6H, a11 - B(A) - H2O
875.086573	12.6	$^{0}C_{56}H_{71}N_{14}O_{31}P_{5}S_{5}$	875.085615	-	-2	d5
876.582999	32.2	$\begin{array}{c} C_{167}H_{204}N_{51}O_{87}P_{15}S_{1}\\ \\ 5\end{array}$	876.583574	0.660	-6	M - 8H - dG, M - 6H - H2O - A, M - 8H - G, M -
877.672545	10.2	$C_{136}H_{167}N_{43}O_{73}P_{13}S_1$	877.673261	0.820	-5	d13 - 7H
879.249058	18.7	³ C ₁₆₇ H ₂₀₄ N ₅₁ O ₈₈ P ₁₅ S ₁	879.249393	0.380	-6	M - 8H - dA, M - 8H - A
881.429630	106.8	⁵ C ₈₆ H ₁₀₃ N ₂₆ O ₄₄ P ₇ S ₇	881.428208	- 1 610	-3	a8 - 4H
882.093894	29.4	$C_{86}H_{103}N_{25}O_{45}P_7S_7$	882.092155	- 1 970	-3	b8 - NH3
884.440406	75.2	$C_{86}H_{104}N_{30}O_{41}P_7S_7$	884.440000	- 0.460	-3	y8 - H2O, z8
887.097547	156.8	$C_{56}H_{71}N_{18}O_{29}P_5S_5$	887.096848	- 0 700	-2	w5
901.758316	1240. 9	$C_{172}H_{209}N_{56}O_{88}P_{15}S_1$	901.758475	0.180	-6	M - 8H
908.420078 909 341915	11.7 32.6	5 C ₈₄ H ₁₀₅ N ₃₀ O ₄₃ P ₈ S ₈ C116H125N26Oc5P45S4	908.421163 909 341245	1.190 -	-3 -4	w8 - OC2H2 a11 - 5H
	02.0	0		0.740	-	

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915.347980	17.5	$C_{116}H_{139}N_{42}O_{57}P_{10}S_1$	915.346862	-	-4	z11 - 5H
919.078457	12.1	$^{0}C_{86}H_{105}N_{26}O_{47}P_8S_8$	919.076950	1.220 - 1.640	-3	d8 - 5H
922.425236	56.4	$C_{86}H_{107}N_{30}O_{44}P_8S_8$	922.424684	- 0.600	-3	w8
943.836443	17.2	$C_{116}H_{142}N_{42}O_{60}P_{11}S_1$	943.835375	- 1 130	-4	w11 - 5H
946.090206	10.9	$^{1}C_{91}H_{110}N_{26}O_{48}P_{8}S_{8}$	946.088297	- 2 020	-3	a9 - 4H
978.120869 978.121170	11.3 76.1	$\begin{array}{l} C_{23}H_{62}N_9O_5P_{14} \\ C_{66}H_{81}N_{16}O_{34}P_5S_5 \end{array}$	978.120608 978.120186	0.270 - 1.010	-1 -2	b6 - H2O, a6
979.118137	14.7	$C_{66}H_{81}N_{15}O_{35}P_5S_5$	979.116107	- 2 070	-2	b6 - NH2
984.069143	84.8	$C_{60}H_{74}N_{18}O_{34}P_6S_6$	984.068789	-	-2	w6 - B(dA) - CH4
987.125573	6.9	$C_{66}H_{83}N_{16}O_{35}P_5S_5$	987.125469	-	-2	b6
989.096010	18.6	$C_{126}H_{151}N_{40}O_{65}P_{11}S_1$	989.095087	-	-4	a12 - 6H
991.107283	28.7	$^{1}C_{96}H_{115}N_{31}O_{48}P_{8}S_{8}$	991.106462	- 0.830	-3	a9 - 4H
992.107347	11.5	$C_{96}H_{116}N_{30}O_{49}P_8S_8$	992.106350	- 1 010	-3	b9 - NH2
1005.45342	6.9	$C_{96}H_{118}N_{35}O_{47}P_8S_8$	1005.45341 4	-	-3	у9
4 1011.64001	9.6	$C_{66}H_{82}N_{23}O_{32}P_5S_5$	4 1011.63994 3	-	-2	у6
1015.18887 7	38.5	$C_{36}H_{45}O_{17}N_{10}P_2S_2$	1015.18863	-	-1	b3
, 1017.58433	5.3	$C_{126}H_{154}N_{40}O_{68}P_{12}S_1$	0 1017.58360	0.240 - 0.720	-4	d12 - 6H
1022.18462	15.6	$^{2}C_{36}H_{42}O_{15}N_{13}P_{2}S_{2}$	0 1022.18454 7	-	-1	y3 - H2O, z3
4 1023.58912	20.7	$C_{126}H_{154}N_{44}O_{66}P_{12}S_1$, 1023.58921 7	0.080	-4	w12 - 6H
2 1026.09280	6.2	$^{2}C_{66}H_{82}N_{16}O_{36}P_{6}S_{6}$, 1026.09193	-	-2	c6 - 3H, d6 - H2O
7 1029.29024 2	12.5	$C_{160}H_{195}O_{84}N_{53}P_{15}S_1$	0 1029.29037	0.830	-5	w15 - 7H, d15 - 7H
2 1035.09807	13.7	$^{5}C_{66}H_{84}N_{16}O_{37}P_{6}S_{6}$	4 1035.09721	-	-2	d6
7 1037.10047 2	27.5	$C_{96}H_{118}N_{35}O_{49}P_9S_9$	2 1037.09863	0.040 - 1.770	-3	w9 - 4H
3 1040.19533 2	54.0	$C_{36}H_{44}O_{16}N_{13}P_2S_2$	1040.19511	- -	-1	уЗ
2 1059.61149	31.9	$C_{66}H_{83}N_{23}O_{34}P_6S_6$	2 1059.61168	0.210	-2	w6
5 1068.85458	9.1	$C_{136}H_{165}N_{43}O_{70}P_{12}S_1$	7 1068.85488	0.280	-4	a13 - 6H
/ 1075.11121	72.7	$^{2}C_{71}H_{88}N_{16}O_{38}P_{6}S_{6}$	2 1075.11032	-	-2	b7 - B(G) - H2O. a7 - B(G)
4 1075.60799	20.2	$C_{136}H_{166}N_{46}O_{69}P_{12}S_1$	0 1075.61041	2.250	-4	y13 - H2O, z13
1082.31048	7.0	${\overset{\scriptscriptstyle 2}{C}}_{172}H_{210}N_{56}O_{88}P_{15}S_1$	1082.31162	1.050	-5	M - 7H
9 1082.51137 4	11.5	${\overset{_{5}}{C}}_{172}H_{211}N_{56}O_{88}P_{15}S_{1}$	1082.51319	1.680	-5	M - 6H
4 1093.12265	6.5	$^{5}C_{36}H_{44}O_{18}N_{10}P_{3}S_{3}$	1093.12155	-	-1	c3 - 2H, d3 - H2O

2 1097.44700	17.6	$C_{106}H_{127}N_{33}O_{54}P_9S_9$	3 1097.44491	1.010 -	-3	a10 - 5H
4 1111.13198	60.8	$C_{36}H_{46}O_{19}N_{10}P_3S_3$	8 1111.13211 0	1.900 0.120	-1	d3
4 1114.12414	5.7	$C_{106}H_{127}N_{40}O_{51}P_9S_9$	9 1114.12384 3	- 0.270	-3	z10 - 4H
4 1118.12819 8	36.1	$C_{36}H_{43}O_{17}N_{13}P_3S_3$	1118.12803	- 0.140	-1	w3 - H2O, x3 - 2H
1118.12844 0	13.1	$C_{36}H_{43}O_{17}N_{13}P_3S_3$	1118.12803 6	- 0.360	-1	w3 - H2O, x3 - 2H
1136.13888 1	204.5	$C_{36}H_{45}O_{18}N_{13}P_3S_3$	1136.13860 0	- 0 250	-1	w3
1149.62985 2	14.1	$C_{76}H_{91}N_{21}O_{39}P_6S_6$	1149.62719 9	- 2 310	-2	a7 - 4H
1150.63526	46.9	$C_{76}H_{93}N_{21}O_{39}P_6S_6$	1150.63502 4	- 0.210	-2	b7 - H2O, a7
1151.77413 2	7.5	$C_{106}H_{129}N_{40}O_{54}P_{10}S_1$	1151.77258 5	- 1 340	-3	w10 - 5H
1162.64610	9.2	$^{0}C_{76}H_{93}N_{25}O_{37}P_{6}S_{6}$	1162.64625	0.130	-2	z7, y7 - H2O
0 1171.65079 7	10.8	$C_{76}H_{95}N_{25}O_{38}P_6S_6$	1171.65154	0.630	-2	у7
, 1191.15830 7	46.8	$C_{41}H_{50}N_{10}O_{20}P_3S_3$	1191.15833 3	0.020	-1	b4 - B(T) - H2O, a4 - B(T), y4 - B(dG) - NH3
1212.45649 9	7.0	$C_{116}H_{139}N_{38}O_{59}P_{10}S_1$	1212.45481 1	- 1 300	-3	a11 - 5H
1216.16485 4	13.1	${}^{0}_{41}H_{49}N_{13}O_{19}P_{3}S_{3}$	1216.16481 6	- 0.030	-1	y4 - B(mC) - H2O, z4 - B(mC)
1218.61785 2	8.1	$C_{76}H_{94}N_{25}O_{40}P_7S_7$	1218.61545 9	- 1.960	-2	w7 - 4H
	26.4	$C_{76}H_{96}N_{25}O_{40}P_7S_7$	1219.62328 4	-	-2	w7
1247.62377 1	12.8	$C_{81}H_{100}N_{21}O_{43}P_7S_7$	- 1247.62515 8	1.110	-2	a8 - B(G), b8 - B(G) - H2O
1258.78289 7	6.6	$C_{116}H_{143}N_{42}O_{60}P_{11}S_1$	1258.78292 5	0.020	-3	w11 - 4H
, 1317.20247 2	71.2	$C_{46}H_{56}N_{12}O_{22}P_3S_3$	1317.20126 1	- 0 920	-1	b4 - H2O, a4
1319.19583	8.8	$C_{46}H_{56}N_{11}O_{23}P_3S_3$	1319.19310 1	-	-1	b4 - NH2
1322.64728	11.4	$C_{86}H_{104}N_{26}O_{44}P_7S_7$	1322.64595	-	-2	a8 - 3H
1335.21256	8.6	$C_{46}H_{58}N_{12}O_{23}P_3S_3$	1335.21182 5	-	-1	b4
1341.22592	9.6	$C_{46}H_{56}N_{16}O_{20}P_3S_3$	1341.22372 7	- 1 640	-1	y4 - H2O, z4
1359.23430	10.2	$C_{46}H_{58}N_{16}O_{21}P_3S_3$, 1359.23429 2	-	-1	y4
1384.13905	9.8	$C_{86}H_{108}N_{30}O_{44}P_8S_8$	1384.14066	1.160	-2	w8
1413.14527	13.1	$C_{46}H_{57}N_{12}O_{24}P_4S_4$	1413.14474 8	- 0 370	-1	d4 - H2O, c4 - 2H
1431.15502 8	6.7	$C_{46}H_{59}N_{12}O_{25}P_4S_4$	1431.15531 2	0.200	-1	d4
- 1455.17738 9	27.3	$C_{46}H_{59}N_{16}O_{23}P_4S_4$		0.270	-1	w4
1637.22440 1	14.4	$C_{56}H_{69}N_{14}O_{28}P_4S_4$	1637.22445 4	0.030	-1	b5 - H2O, a5

1650.14345 3	9.0	$C_{51}H_{65}N_{15}O_{28}P_5S_5$	1650.14206 1	- 0 840	-1	w5 - B(mC)
1775.20049 6	11.7	$C_{56}H_{72}N_{18}O_{29}P_5S_5$	1775.20097 3	0.270	-1	w5
-			Abs mean error	0.703		
			Abs mean std dev	0.616		

Measured <i>mz</i>	S/N	Elemental Composition	Theoretical <i>mz</i>	Error (ppm)	Charge	Assignment
319.011609	21.6	$C_{31}H_{36}O_{19}N_4P_3S_3$	319.012174	1.770	-3	d3 - B(dA) - NH3
319.016031	217.3	C ₁₀ H ₁₃ N ₂ O ₆ PS	319.015918	-0.350	-1	bTx
327.019861	40.3	$C_{31}H_{36}O_{17}N_8P_3S_3$	327.019846	-0.050	-3	d3 - 5H, x3 - 4H, w3 - B(dA) - H2O
343.014726	149.6	C ₁₀ H ₁₁ N ₅ O ₅ PS	343.014575	-0.440	-1	bGy
344.022551	141.0	$C_{10}H_{12}N_5O_5PS$	344.022400	-0.440	-1	cGy
360.042633	26.3	$C_{12}H_{15}O_6N_3PS$	360.042467	-0.460	-1	x1 - 2H, c1 - 2H, d1 - H2O, w1 - H2O
361.026830	28.4	$C_{24}H_{28}O_{14}N_4P_2S_2$	361.026757	-0.200	-2	d2 - NH3
370.038402	32.9	$C_{61}H_{71}N_{18}O_{30}P_5S_5$	370.038161	-0.650	-5	z6 - 6H
377.045457	27.1	$C_{49}H_{60}N_{16}O_{24}P_4S_4$	377.045541	0.220	-4	y5 - B(T) -
270 052260	96 1		270 052022	0 620	1	OC2H2 d1_w1
378.053268 386.033273 398.982483 414.959681 423.988989 439.966411 450.004856 465.981949	34.6 154.5 99.6 94.1 60.3 99.1 87.7	C ₁₂ Π ₁₇ O7N ₃ FS	378.033032	-0.620	-1	G1, W1
484.388097 512.996699	261.1 245.1	$C_{46}H_{57}N_{16}O_{23}P_4S_4$	484.387925	-0.360	-3	w4
529.302659 538.003140	100.9 126.7	$C_{66}H_{81}N_{23}O_{34}P_6S_6$	529.302342	-0.600	-4	w6
540.853737	61.9	C172H207N56O88P15S15	540.853740	0.010	-10	M-10H
554.559063	60.4	$C_{36}H_{44}O_{19}N_{10}P_3S_3$	554.558782	-0.510	-2	d3 - 3H
567.566334	132.7	C ₃₆ H ₄₄ O ₁₈ N ₁₃ P ₃ S ₃	567.565936	-0.700	-2	w3
591.062641	65.9	$C_{56}H_{70}N_{18}O_{29}P_5S_5$	591.062323	-0.540	-3	w5
595.076172	43.2	$C_{41}H_{49}N_{10}O_{20}P_3S_3$	595.075802	-0.620	-2	y4 - B(dG) - NH3, b4 - B(T) - H2O, a4 - B(T)
601.060434	282.4	$C_{172}H_{208}N_{56}O_{88}P_{15}S_{15}$	601.060519	0.140	-9	M-9H
603.725617	140.4	$C_{61}H_{72}N_{14}O_{31}P_5S_5$	603.726534	1.520	-3	a6 - B(T) - H2O
604.059080	146.5	$C_{59}H_{75}N_{11}O_{35}P_5S_5$	604.058021	-1.750	-3	b6 - B(dA) - C2H2
606.055353	63.8	$C_{61}H_{73}N_{11}O_{34}P_5S_5$	606.054500	-1.410	-3	
606.388959	24.3	$C_{115}H_{136}N_{38}O_{60}P_{10}S_{10}$	606.389586	1.030	-6	DTT - CH4
609.308611	130.8	$C_{76}H_{94}N_{25}O_{40}P_7S_7$	609.308141	-0.770	-4	w/
609.559517	78.2	$C_{116}H_{135}N_{42}O_{57}P_{10}S_{10}$	609.559541	0.040	-6	
610.058898	28.4	$C_{61}H_{73}N_{13}O_{33}P_5S_5$	610.058244	-1.070	-3	a6 - B(dC), b6 - B(dC) - H2O, b6 - B(T) - NH3
622.058333	21.4	$C_{96}H_{117}N_{35}O_{49}P_9S_9$	622.057945	-0.620	-5	w9
629.055744	16.1	$C_{116}H_{141}N_{42}O_{60}P_{11}S_{11}$	629.055795	0.080	-6	w11
638.056137	13.1	$C_{100}H_{117}N_{35}O_{51}P_9S_9$	638.055911	-0.350	-5	z10 - B(A) - CH4
639.040176	29.4		044 440050	0.040		h0
644.143859	27.3	$U_{24}H_{31}U_{12}N_5PS$	644.143852	-0.010	-1	
647.043640	23.1	$C_{41}H_{52}N_7O_{25}P_4S_4$	647.043132	-0.780	-2	04 - 3H
651.409120	19.7	$C_{66}H_{79}N_{16}O_{34}P_5S_5$	651.408607	-0.790	-3	ab - 4H
651.744654	42.3	$C_{66}H_{80}N_{16}O_{34}P_5S_5$	651./44548	-0.160	-3	00 - H2U, 20
050.048613	11./	$U_{80}H_{96}N_{28}U_{42}P_8S_8$	050.048274	-0.520	-4	wo-в(т)-СН4
057.593725	251.9	$C_{46}H_{54}N_{12}O_{22}P_3S_3$	057.593354	-0.560	-2	a4 - 3⊓ b4 ⊔20 - 4
658.588802	143.0	u ₄₆ H ₅₅ N ₁₂ U ₂₂ P ₃ S ₃ C ₄₆ H ₅₄ N ₁₁ O ₂₃ P ₃ S ₃	658.589000	0.300	-2 -2	b4 - NH3

Table S9 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the autocorrelation line of danvatirsen by 2D-EDD-MS.
658.598913	49.3					
659.092455	11.5	$C_{46}H_{55}N_{11}O_{23}P_3S_3$	659.092912	0.690	-2	b4 - NH2
660.819106	24.9	C ₈₆ H ₁₀₂ N ₂₆ O ₄₄ P ₇ S ₇	660.819337	0.350	-4	a8 - 5H
661.070612	38.3	$C_{86}H_{103}N_{26}O_{44}P_7S_7$	661.071293	1.030	-4	a8, b8 - H2O
661.570282	16.6	$C_{86}H_{103}N_{25}O_{45}P_7S_7$	661.569390	-1.350	-4	b8 - NH2
664.046582	95.9					
665.051031	11.7	$C_{143}H_{171}O_{75}N_{49}P_{14}S_{14}$	665.050479	-0.830	-7	w14 - 10H
668.552340	14.1					
670.108765	15.8	$C_{46}H_{55}N_{16}O_{20}P_3S_3$	670.108499	-0.400	-2	y4 - H2O, z4
675.198922	10.0	C ₁₄₈ H ₁₇₈ O ₇₇ N ₄₇ P ₁₄ S ₁₄	675.198830	-0.140	-7	c14 - NH2
676.319005	461.9	$C_{172}H_{209}N_{56}O_{88}P_{15}S_{15}$	676.318994	-0.020	-8	M-8H
677.694657	46.5					
679.192056	400.0					
682.393701	11.6	$C_{126}H_{154}N_{44}O_{66}P_{12}S_{12}$	682.393085	-0.900	-6	W12
682.814854	13.8	$C_{86}H_{103}N_{30}O_{42}P_8S_8$	682.813505	-1.970	-4	
683.059470	14.9	$C_{86}H_{102}N_{29}O_{43}P_8S_8$	683.059509	0.060	-4	
083.009009	0.3 110 F	$C_{85}\Pi_{102}N_{30}O_{43}P_8S_8$	083.000140	0.920	-4	
004.000317	74.0	$C_{106}\Pi_{126}\Pi_{40}O_{52}\Pi_{10}O_$	004.001110 694.550006	1.100	-5 4	w8 - C2H4
004.009700 695.059575	14.2	$C_{84}\Pi_{102}N_{30}O_{44}\Gamma_8S_8$	695 057202	-1.020	-4	d8 - H2O - c8 -
005.050545	10.9	C86H104N26C46F8S8	005.057502	-1.010	-4	5H
685.805414	8.8	$C_{85}H_{103}N_{26}O_{47}P_8S_8$	685.804074	-1.950	-4	d8 - CH3
689.729726	12.0	$C_{66}H_{83}N_{16}O_{37}P_6S_6$	689.729232	-0.720	-3	d6
691.063386	10.4	$C_{106}H_{129}N_{40}O_{54}P_{10}S_{10}$	691.063771	0.560	-5	w10
691.567090	68.1	$C_{86}H_{106}N_{30}O_{44}P_8S_8$	691.566831	-0.370	-4	w8
692.067493	54.5	$C_{64}H_{80}N_{23}O_{33}P_6S_6$	692.068511	1.470	-3	w6 - OC2H2
706.072783	27.2	$C_{66}H_{82}N_{23}O_{34}P_6S_6$	706.072215	-0.800	-3	w6
712.736751	8.1	$C_{134}H_{164}N_{46}O_{69}P_{12}S_{12}$	712.737851	1.540	-6	y13 - OC2H2
715.074533	23.5	$C_{46}H_{58}N_{12}O_{25}P_4S_4$	715.074292	-0.340	-2	d4
722.076030	21.3	$C_{24}H_{30}O_{13}N_5P_2S_2$	722.076226	0.270	-1	d2 - H2O, c2 - 2H
727.085857	41.7	C ₄₆ H ₅₈ N ₁₆ O ₂₃ P ₄ S ₄	727.085525	-0.460	-2	w4
727.271462	7.1	C ₁₁₆ H ₁₃₈ N ₃₈ O ₅₉ P ₁₀ S ₁₀	727.271541	0.110	-5	a11 - 6H
727.472231	16.2	$C_{116}H_{139}N_{38}O_{59}P_{10}S_{10}$	727.473106	1.200	-5	a11, b11 - H2O
727.872499	13.5	$C_{116}H_{139}N_{37}O_{60}P_{10}S_{10}$	727.871584	-1.260	-5	b11 - NH2
732.071730	5.4	$C_{24}H_{28}O_{12}N_7P_2S_2$	732.071809	0.110	-1	x2 - NH2
740.087631	18.2	$C_{24}H_{32}O_{14}N_5P_2S_2$	740.087340	-0.390	-1	d2
743.078355	13.6	$C_{96}H_{114}N_{31}O_{48}P_8S_8$	743.078164	-0.260	-4	a9 - 5H
743.329545	41.9	$C_{96}H_{115}N_{31}O_{48}P_8S_8$	743.329984	0.590	-4	b9 - H2O, a9
743.580405	26.4	$C_{49}H_{61}N_{11}O_{27}P_4S_4$	743.579407	-1.340	-2	b5 - B(dC) - OC2H2
747.083523	17.6	$C_{50}H_{60}N_{13}O_{25}P_4S_4$	747.083654	0.180	-2	25 - B(dG) - CH3
747.569553	12.6	$C_{51}H_{59}N_{10}O_{27}P_4S_4$	747.569771	0.290	-2	a5 - B(dC) - NH2
747.903351	6.0	$C_{141}H_{174}O_{75}N_{43}P_{13}S_{13}$	747.902000	-1.810	-6	b14 - B(dA) - OC2H2
749.076596	8.0	$C_{24}H_{29}O_{13}N_7P_2S_2$	749.075098	-2.000	-1	w2 - NH2
749.335900	13.0	$C_{96}H_{115}N_{35}O_{46}P_8S_8$	749.335737	-0.220	-4	z9, y9 - H2O
749.585787	12.4	$C_{49}H_{61}N_{13}O_{26}P_4S_4$	749.585024	-1.020	-2	y5 - B(dG) - C2H4, z5 -
753.786011	26.1	$C_{167}H_{205}N_{51}O_{88}P_{15}S_{15}$	753.786390	0.500	-7	B(dA) - C2H2 M - 7H - dA, M -
754.786605	16.5	$C_{167}H_{202}N_{54}O_{86}P_{15}S_{15}$	754.785885	-0.950	-7	M - 9H - T, M -
754.929698	12.4	$C_{167}H_{203}N_{54}O_{86}P_{15}S_{15}$	754.929782	0.110	-7	M - 8H - dU, M
755.088803	6.4	$C_{51}H_{62}N_{12}O_{26}P_4S_4$	755.087399	-1.860	-2	b5 - B(T) -
						H2O, y5 - B(dG) - NH3
						a5 - B(T)
756.090214	18.6	$C_{50}H_{62}N_{13}O_{26}P_4S_4$	756.088936	-1.690	-2	y5 - B(dG) - CH3
756.232424	9.0	$C_{143}H_{172}O_{75}N_{45}P_{13}S_{13}$	756.233659	1.630	-6	b14 - 8H, y14 - B(dA) - NH3

756.376017	6.8	C ₇₁ H ₈₄ N ₁₈ O ₄₀ P ₇ S ₇	756.377233	1.610	-3	c7 - 6H
757.068598	12.1	$C_{143}H_{169}O_{72}N_{49}P_{13}S_{13}$	757.067763	-1.100	-6	z14 - 9H
759.087846	6.9	C ₅₁ H ₆₀ N ₁₅ O ₂₄ P ₄ S ₄	759.088997	1.520	-2	z5 - B(T) - NH2
765.094292	36.5	C ₂₄ H ₃₁ O ₁₃ N ₈ P ₂ S ₂	765.093822	-0.620	-1	w2
766.418642	23.3	$C_{76}H_{91}N_{21}O_{39}P_6S_6$	766.418499	-0.190	-3	a7 - 4H
766.754132	81.9	$C_{76}H_{92}N_{21}O_{30}P_6S_6$	766.754257	0.160	-3	a7, b7 - H2O
768.088457	7.1	$C_{50}H_{60}N_{16}O_{25}P_4S_4$	768.088265	-0.250	-2	y5 - B(T) - CH4
771.227056	21.3	$C_{142}H_{171}O_{74}N_{49}P_{14}S_{14}$	771.226315	-0.960	-6	x14 - B(T) -
772 070000	245 0		772 070000	0.040	7	
774.223221	315.8 145.8	$C_{172}H_{210}N_{56}O_{88}P_{15}S_{15}$ $C_{142}H_{171}O_{76}N_{48}P_{14}S_{14}$	774.224017	1.030	-7 -6	w14 - B(mC) -
774 760340	13.6	$C_{72}H_{22}N_{22}O_{27}P_{2}S_{2}$	774 761746	1 810	-3	v7 - H2O, z7
775 097355	76	$C_{r_4}H_{00}N_{40}O_{0}P_4S_4$	775 096090	-1 630	-2	v5 - 4H
777 077618	224.0	$C_{4,40}$ H _{4,70} O ₇₀ N ₄₀ P ₄₀ S ₄₀	777 076902	-0.920	-6	b14 - 8H
777 824516	224.0	C_{148} $1_{1/9}$ C_{16} 4_{48} 1_{3} C_{13}	777 824250	-0.340	_4	w9
778 07/025	16.3	$C_{96} H_{118} R_{35} C_{49} R_{9} C_{90}$	778 07/018	-0.040	-4	714 - 9H
782 060000	12.0	$C \square N O D S$	792 069292	-0.010	-0	a10 - B(A) -
783.009009	13.0	C991 1 ₁₂₁ N28 C54 F 9 S9	783.008383	-0.000	-4	C2H2
785.066365	22.3	C ₇₄ H ₉₂ N ₂₁ O ₄₀ P ₇ S ₇	785.067840	1.880	-3	c7 - OC2H2
791.276129	6.9	$C_{126}H_{151}N_{40}O_{65}P_{11}S_{11}$	791.276180	0.070	-5	a12 - 6H
791.476939	27.1	$C_{126}H_{152}N_{40}O_{65}P_{11}S_{11}$	791.477745	1.020	-5	b12 - H2O, a12
791.877687	26.1	$C_{126}H_{152}N_{39}O_{66}P_{11}S_{11}$	791.876223	-1.850	-5	b12 - NH2
804.739029	8.5	C ₇₆ H ₉₅ N ₂₁ O ₄₂ P ₇ S ₇	804.738941	-0.110	-3	d7
805.073927	8.4	$C_{100}H_{119}N_{37}O_{51}P_9S_9$	805.075064	1.410	-4	y10 - B(mC) - CH3
812.746917	40.4	$C_{76}H_{95}N_{25}O_{40}P_7S_7$	812.746613	-0.370	-3	w7
817.605408	36.4	$C_{56}H_{67}N_{14}O_{28}P_4S_4$	817.604950	-0.560	-2	a5 - 3H
818.108472	83.1 32 7	$C_{56}H_{68}N_{14}O_{28}P_4S_4$	818.108589	0.140	-2	b5 - H2O, a5
819 073146	39.5	CupeHurrNu OpePueSue	819 073158	0.010	-5	w12
810 873555	48.5	$C_{126}H_{155}H_{44}C_{66}H_{12}C_{12}$	819 872678	-1 070	-5	a13 - B(A) -
010.070000	40.0		010.072070	-1.070	-0	OC2H2, a13 - B(G) - C2H2
823.084380	6.1	C ₁₀₆ H ₁₂₇ N ₃₃ O ₅₄ P ₉ S ₉	823.083963	-0.510	-4	a10 - 5H
823.335441	24.8	C ₁₀₆ H ₁₂₈ N ₃₃ O ₅₄ P ₉ S ₉	823.335782	0.410	-4	a10, b10 - H2O
823.834661	31.6	C ₁₀₆ H ₁₂₈ N ₃₂ O ₅₅ P ₉ S ₉	823.833879	-0.950	-4	b10 - NH2
824.469533	7.3	$C_{129}H_{156}N_{41}O_{68}P_{12}S_{12}$	824.470735	1.460	-5	z13 - B(G) -
						C2H4, a13 - B(T) - C2H4
827.062913	10.1	$C_{155}H_{187}O_{82}N_{47}P_{15}S_{15}$	827.063591	0.820	-6	x15 - B(G) - NH3. c15 -
						B(dG) - NH3
828.563397	8.8	$C_{100}H_{120}N_{38}O_{52}P_{10}S_{10}$	828.563113	-0.340	-4	w10 - B(T) - CH4
829.082651	7.1	C ₈₀ H ₉₆ N ₂₅ O ₄₀ P ₇ S ₇	829.082555	-0.120	-3	z8 - B(G) - CH3
830.120195	46.1	$C_{56}H_{68}N_{18}O_{26}P_4S_4$	830.120096	-0.120	-2	y5 - H2O, z5
835.593455	6.6	$C_{106}H_{127}N_{40}O_{51}P_9S_9$	835.593157	-0.360	-4	z10, y10 - H2O
837.081668	6.8	$C_{79}H_{98}N_{24}O_{43}P_7S_7$	837.081662	-0.010	-3	b8 - B(T) - C2H2
839.124861	5.5	$C_{56}H_{70}N_{18}O_{27}P_4S_4$	839.125105	0.290	-2	y5
840.095850	12.7	$C_{106}H_{129}N_{40}O_{52}P_9S_9$	840.095798	-0.060	-4	y10
852.074567	6.3	$C_{160}H_{193}O_{82}N_{53}P_{15}S_{15}$	852.074581	0.020	-6	c15 - H2O, x15 - H2O
855.284879	5.8	$C_{136}H_{166}N_{43}O_{70}P_{12}S_{12}$	855.285580	0.820	-5	a13, b13 - H2O
860.286765	34.6	C ₁₃₆ H ₁₆₅ N ₄₆ O ₆₉ P ₁₂ S ₁₂	860.286877	0.130	-5	z13, y13 - H2O
860.484189	56.8	$C_{136}H_{164}N_{45}O_{70}P_{12}S_{12}$	860.483790	-0.460	-5	y13 - NH3
864.081945	11.7	$C_{106}H_{130}N_{40}O_{54}P_{10}S_{10}$	864.081669	-0.320	-4	w10
868.076643	6.9	$C_{110}H_{132}N_{33}O_{58}P_{10}S_{10}$	868.075117	-1.760	-4	a11 - B(G) -
975 096203	16 7		975 095990	0.360	2	CH3 d5
977 095264	10.7 Q 7	0561 1711N14U31F5O5 С Ц N О РС	010.000009 977 00101E	-0.300	-2	чо х5 ₋ 5Н
077 E0010E	0.1 7 0	0561 1671 N18028 Г505 С Ц N О РС	011.004010 977 507007	0 200	-2	χ5 - <i>Δ</i> Η
077.000190 991.095550	1.3 5.4	056П68IN18U28F5O5 С Ц N О Р С	011.001921 991.097060	-0.300	-2	M - 6H - T M -
001.000000	5.4	01671 12051N54086P15015	001.007202	1.940	-0	6H - dU
881.250438	6.8	C ₁₆₇ H ₂₀₄ N ₅₃ O ₈₇ P ₁₅ S ₁₅	881.251265	0.940	-6	M - 6H - dC, M

						- 6H - mC
881.429088	58.8	$C_{86}H_{103}N_{26}O_{44}P_7S_7$	881.428391	-0.790	-3	a8 - 4H
881.583007	5.4	$C_{109}H_{132}N_{40}O_{56}P_{10}S_{10}$	881.583039	0.040	-4	у11 - В(Т) - С2Н4
881 763510	68 2	$C_{00}H_{404}N_{00}O_{44}P_7S_7$	881 764149	0 720	-3	a8, b8 - H2O
883 431617	8.0	$C_{86}H_{104}N_{26}O_{44}P_7S_7$	883 432175	0.630	-3	z8 - 6H
883.578160	6.0	$C_{111}H_{120}N_{20}O_{56}P_{10}S_{10}$	883.578221	0.070	-4	z11 - 7H
884.440325	50.4	$C_{86}H_{104}N_{30}O_{41}P_7S_7$	884.440183	-0.160	-3	y8 - H2O, z8
887.097332	97.3	$C_{56}H_{71}N_{18}O_{20}P_5S_5$	887.097122	-0.240	-2	w5
887.598954	86.1	- 30: 71: 10 - 29: 3 - 3			_	
901.757653	7.1	C ₁₇₂ H ₂₀₉ N ₅₆ O ₈₈ P ₁₅ S ₁₅	901.758475	0.910	-6	M - 8H
901.924796	19.4	$C_{172}H_{210}N_{56}O_{88}P_{15}S_{15}$	901.926446	1.830	-6	M - 7H
902.094315	188.1	C ₁₇₂ H ₂₁₁ N ₅₆ O ₈₈ P ₁₅ S ₁₅	902.094417	0.110	-6	M - 6H
905.588478	6.9	$C_{116}H_{138}N_{37}O_{59}P_{10}S_{10}$	905.588520	0.050	-4	a11 - NH2
906.092077	220.4	$C_{61}H_{73}N_{14}O_{31}P_5S_5$	906.093440	1.500	-2	a6 - B(T) - H2O
906.564274	9.1	$C_{111}H_{135}N_{35}O_{61}P_{11}S_{11}$	906.565030	0.830	-4	d11 - 5H
906.592128	223.2	$C_{59}H_{76}N_{11}O_{35}P_5S_5$	906.590670	-1.610	-2	b6 - B(dA) -
007 502153	71		007 502067	0 000	4	62H2 b11 - C2H2
907.392133	7.1 285.7	$C_{114} I_{140} I_{38} O_{60} F_{10} O_{10}$	907.392007 000 085002	-0.090	-4 -5	z14 - 6H
909.000555	94 N	$C_{143} + 1_{172} + 0_{72} + 4_{9} + 1_{3} + 0_{13}$	909.000902	-0.300	-0	a6 - 3H
910.009307	62	C_{61} C_{75} C_{11} C_{34} C_{505}	910.009300 911 749279	1 490	-2	x8 - CH3
913 082720	0.2 61.6	$C_{85} H_{103} N_{30} C_{43} R_{8} C_{8}$	913 081100	-1 770	-3	w8 - C2H4
914 081927	5.3	$C_{84}H_{103}H_{30}C_{44}H_{8}C_{8}$	914 081437	-0.540	-3	c8
914 741032	13.0	$C_{86}H_{106}C_{26}O_{46}B_{8}O_{8}O_{4}$	914 741008	-0.030	-3	d8 - CH3
916.578746	15.9	$C_{60}H_{72}N_{12}O_{24}P_5S_5$	916.580362	1.760	-2	b6 - B(dC) -
		00. 72. 13 0 34. 505	0.000000		_	CH4
918.740473	9.4	C ₈₆ H ₁₀₄ N ₂₆ O ₄₇ P ₈ S ₈	918.741008	0.580	-3	d8 - 6H
919.076008	19.9	$C_{86}H_{105}N_{26}O_{47}P_8S_8$	919.076950	1.020	-3	d8 - 5H
919.749921	5.4	C ₈₆ H ₁₀₇ N ₂₆ O ₄₇ P ₈ S ₈	919.749017	-0.980	-3	d8
922.424960	100.3	$C_{86}H_{107}N_{30}O_{44}P_8S_8$	922.424867	-0.100	-3	W8
924.092163	13.3	$C_{61}H_{75}N_{13}O_{34}P_5S_5$	924.092100	-0.070	-2	D6 - 3H
944.087042	12.0	$C_{116}H_{143}N_{42}O_{60}P_{11}S_{11}$	944.087331	0.310	-4	W11
945.088139	11.1	$C_{89}H_{107}N_{30}O_{46}P_8S_8$	945.088144	0.010	-3	29 - B(A) - C2H4
946.424307	8.4	C01H111N26O48P8S8	946.424239	-0.070	-3	a9 - B(A), b9 -
						B(A) - H2O
950.083168	8.4	$C_{91}H_{108}N_{27}O_{48}P_8S_8$	950.084105	0.990	-3	b9 - B(dC) - NH3
977.617343	34.0	C66H80N16O34P5S5	977.616548	-0.810	-2	a6 - 3H
978.119841	86.4	$C_{66}H_{81}N_{16}O_{34}P_5S_5$	978.120186	0.350	-2	b6 - H2O, a6
984.069909	15.4	$C_{60}H_{74}N_{18}O_{34}P_6S_6$	984.069063	-0.860	-2	w6 - B(dA) -
						CH4
985.072345	6.6	$C_{90}H_{108}N_{32}O_{47}P_9S_9$	985.072868	0.530	-3	x9 - B(mC) - CH3
989.346629	5.2	C126H152N40O65P11S11	989.347044	0.420	-4	a12 - 5H
990.097992	19.1	$C_{126}H_{153}N_{30}O_{66}P_{11}S_{11}$	990.097097	-0.900	-4	b12 - NH2
991.106680	12.8	$C_{96}H_{115}N_{31}O_{48}P_8S_8$	991.106645	-0.040	-3	a9 - 4H
991.441706	32.2	$C_{96}H_{116}N_{31}O_{48}P_8S_8$	991.442404	0.700	-3	b9 - H2O, a9
992.073403	10.4	$C_{121}H_{146}N_{41}O_{65}P_{12}S_{12}$	992.072670	-0.740	-4	w12 - 7H
993.081008	15.4					
996.588782	8.4	$C_{61}H_{77}N_{21}O_{32}P_6S_6$	996.590223	1.450	-2	w6 - B(T)
999.451200	31.3	C ₉₆ H ₁₁₆ N ₃₅ O ₄₆ P ₈ S ₈	999.450076	-1.120	-3	y9 - H2O, z9
1002.132275	8.7	$C_{66}H_{79}N_{23}O_{31}P_5S_5$	1002.131022	-1.250	-2	z6 - 3H
1002.634141	19.9	$C_{66}H_{80}N_{23}O_{31}P_5S_5$	1002.634661	0.520	-2	z6, y6 - H2O
1010.080030	8.4	$C_{125}H_{152}N_{40}O_{67}P_{12}S_{12}$	1010.080959	0.920	-4	c12 - CH3
1011.640641	9.4	$C_{66}H_{82}N_{23}O_{32}P_5S_5$	1011.640217	-0.420	-2	y6
1015.190122	6.9	$C_{36}H_{45}O_{17}N_{10}P_2S_2$	1015.189179	-0.930	-1	b3
1022.183983	11.2	$C_{36}H_{42}O_{15}N_{13}P_2S_2$	1022.184547	0.550	-1	y3 - H2O, z3
1024.093613	16.8	$C_{126}H_{156}N_{44}O_{66}P_{12}S_{12}$	1024.093267	-0.340	-4	w12
1025.094590	32.0	$C_{129}H_{160}N_{38}O_{69}P_{12}S_{12}$	1025.092667	-1.880	-4	a13 - B(A) - OC2H2 - 13
						B(G) - C2H2
1030.839351	7.2	$C_{129}H_{157}N_{41}O_{68}P_{12}S_{12}$	1030.840238	0.860	-4	z13 - B(G) -
						C2H4, a13 -

						B(T) - C2H4
1035.098226	19.5	$C_{66}H_{84}N_{16}O_{37}P_6S_6$	1035.097486	-0.710	-2	d6
1037.099635	6.8	$C_{96}H_{118}N_{35}O_{49}P_9S_9$	1037.098818	-0.790	-3	w9 - 4H
1037.434876	39.4	$C_{96}H_{119}N_{35}O_{49}P_9S_9$	1037.434760	-0.110	-3	w9
1038.100170	56.6	$C_{129}H_{160}N_{44}O_{67}P_{12}S_{12}$	1038.099820	-0.340	-4	у13 - B(T) - ОС2Н2
1040 196102	20.4		1040 195661	-0 420	-1	v3
1051.086725	12.9	$C_{100}H_{110}N_{20}O_{52}P_0S_0$	1051.086731	0.010	-3	a10 - B(dC) -
		• 100. 1118. 30 • 33. 9 • 9			•	CH4
1052.096373	13.2	$C_{165}H_{201}N_{53}O_{87}P_{15}S_{15}$	1052.096713	0.320	-5	M - 5H - C2H4 - dC, M - 5H -
4050 504007	0.4			0.050	-	C2H4 - mC
1052.504927	6.1	$C_{167}H_{207}N_{51}O_{87}P_{15}S_{15}$	1052.504874	-0.050	-5	M - 5H - G, M - 5H - dG
1056.101745	5.7	$C_{101}H_{123}N_{31}O_{52}P_9S_9$	1056.102493	0.710	-3	b10 - B(T) -
1056.903430	6.3	C ₁₆₇ H ₂₀₃ N ₅₄ O ₈₆ P ₁₅ S ₁₅	1056.901585	-1.750	-5	M - 8H - dU, M
4050 400000	0.4		4050 400040	4 450	0	- 8H - T
1059.109268	8.4	$C_{66}H_{82}N_{23}O_{34}P_6S_6$	1059.108048	-1.150	-2	WO - 3H
1059.612243	01.7	$C_{66}H_{83}N_{23}O_{34}P_6S_6$	1059.611961	-0.270	-2	WU
1069.358294	12.3	C ₁₃₆ H ₁₆₇ N ₄₃ O ₇₀ P ₁₂ S ₁₂	1069.358794	0.470	-4	D13 - H2U
1069.858925	21.7	$C_{136}H_{167}N_{42}O_{71}P_{12}S_{12}$	1069.856892	-1.900	-4	
1075.110815	59.2	C ₇₁ H ₈₈ N ₁₆ O ₃₈ P ₆ S ₆	1075.110594	-0.210	-2	b7 - B(G) -
1075 611640	100.2		1075 610552	1 010	1	H2O, a7 - B(G)
1075.011040	100.2	$C_{136}\Pi_{166}\Pi_{46}O_{69}P_{12}S_{12}$	1075.010552	-1.010	-4	у13-1120, 213 M оц
1082.107996	22.4	C ₁₇₂ H ₂₀₉ N ₅₆ O ₈₈ P ₁₅ S ₁₅	1082.110061	1.910	-5	
1082.309583	14.7	$C_{172}H_{210}N_{56}O_{88}P_{15}S_{15}$	1082.311626	1.890	-5	M - 7H
1082.512783	41.3	$C_{172}H_{211}N_{56}O_{88}P_{15}S_{15}$	1082.513191	0.380	-5	M - 6H
1082.714713	356.6	$C_{172}H_{212}N_{56}O_{88}P_{15}S_{15}$	1082.714756	0.040	-5	M - 5H
1082./151/9	250.4		1004 115070	0.070	2	b7 B(C)
1004.115955	352.1	$C_{71}\Pi_{90}N_{16}O_{39}P_6S_6$	1004.110070	-0.070	-2	
1085.118256	15.6	$C_{34}H_{44}O_{19}N_{10}P_3S_3$	1085.117017	-1.140	-1	
1087.111447	187.4	$C_{71}H_{86}N_{19}O_{37}P_6S_6$	1087.109922	-1.400	-2	a7 - 3H, z7 - B(dA) - NH2
1088 112530	351 1	CHNOP-S-	1088 111/50		_2	v7 - B(G) - CH4
1000.112555	220.2	$C \square N \cap DS$	1000.111409	-0.990	2	b7 - 4H
1091.105505	215 A	$C_{71}I_{88}I_{16}O_{40}F_6O_6$	1091.103308	-0.030	-2	z7 - B(mC) -
1092.107710	213.4	0711 1841 N21 O36F 6O6	1092.107714	0.000	-2	NH2
1095.101352	213.3	$C_{35}H_{42}O_{19}N_{10}P_3S_3$	1095.101367	0.010	-1	d3 - CH4
1096.101538	85.3	$C_{71}H_{86}N_{18}O_{39}P_6S_6$	1096.103026	1.360	-2	b7 - 4H
1097.781767	23.2	C ₁₀₆ H ₁₂₈ N ₃₃ O ₅₄ P ₉ S ₉	1097.781043	-0.660	-3	a10 - 4H
1098.116546	64.2	C106H129N33O54P9S9	1098.116802	0.230	-3	b10 - H2O, a10
1099.094584	41.2	C136H165N46O71P13S13	1099.092511	-1.890	-4	x13 - 7H
1102.151792	22.5					
1111.133940	75.4	$C_{36}H_{46}O_{19}N_{10}P_3S_3$	1111.132668	-1.140	-1	d3
1114.459680	27.5	C106H128N40O51P9S9	1114.459785	0.090	-3	y10 - H2O, z10
1136,139998	292.1	$C_{36}H_{45}O_{18}N_{13}P_3S_3$	1136.139149	-0.750	-1	w3
1137.142785	101.7					
1150.131743	35.5	$C_{39}H_{47}N_9O_{20}P_3S_3$	1150.131784	0.040	-1	a4 - B(dC) -
					-	OC2H2
1150.635111	62.9	$C_{76}H_{93}N_{21}O_{39}P_6S_6$	1150.635024	-0.080	-2	b7 - H2O, a7
1152.444294	22.1	C ₁₀₆ H ₁₃₁ N ₄₀ O ₅₄ P ₁₀ S ₁₀	1152.444469	0.150	-3	w10
1162.648561	22.4	$C_{76}H_{93}N_{25}O_{37}P_6S_6$	1162.646532	-1.740	-2	z7, y7 - H2O
1171.651965	8.4	$C_{76}H_{95}N_{25}O_{38}P_6S_6$	1171.651814	-0.130	-2	у7
1191.160843	13.9	$C_{41}H_{50}N_{10}O_{20}P_3S_3$	1191.158882	-1.650	-1	b4 - B(T) -
						H2O, a4 - B(T),
						у4 - В(dG) - NH3
1010 780010	0.1		1010 700753	1 270	3	a11 - 4H
1212.109212	J. I 11 /		1212.180100	1 1 1 1 0	-0	h11 - NH2
1213.192100	11.4	$O_{116} \Pi_{141} \Pi_{37} O_{60} \Gamma_{10} O_{10}$	1213.190024	-1.110	-3	w7
1219.024330	30.4 40.4		1219.023558	-0.040	-2	₩1 711 GU
1220.124821	40.4	$U_{116}H_{138}N_{42}U_{57}P_{10}S_{10}$	1220.126358	1.260	-3	211-0H
1247.624622	16.6	$C_{81}H_{100}N_{21}O_{43}P_7S_7$	1247.625158	0.430	-2	ao - B(G), bo - B(G) - H2O
1248,127243	19.8	$C_{70}H_{00}N_{24}O_{40}P_7S_7$	1248,128399	0.930	-2	b8 - B(T) -
		-13. 33. 24 42. 101		2.000	-	OC2H2

1259.118979	31.6	$C_{116}H_{144}N_{42}O_{60}P_{11}S_{11}$	1259.119050	0.060	-3	w11
1266.781359	13.4	$C_{119}H_{149}N_{35}O_{65}P_{11}S_{11}$	1266.782927	1.240	-3	b12 - B(A) - OC2H2
1272.102168	11.6	$C_{40}H_{50}N_{11}O_{21}P_4S_4$	1272.102155	-0.010	-1	x4 - B(dG) - CH3
1272.770892	10.5	$C_{120}H_{143}N_{37}O_{64}P_{11}S_{11}$	1272.771022	0.100	-3	a12 - B(dC) - CH4
1316.194430	87.0	$C_{46}H_{55}N_{12}O_{22}P_3S_3$	1316.193985	-0.340	-1	a4 - 2H
1317.200900	151.6	$C_{46}H_{56}N_{12}O_{22}P_3S_3$	1317.201261	0.270	-1	b4 - H2O, a4
1318.204373	55.0				-	0.011
1322.646805	17.8	$C_{86}H_{104}N_{26}O_{44}P_7S_7$	1322.646224	-0.440	-2	a8 - 3H
1323.149057	36.9	$C_{86}H_{105}N_{26}O_{44}P_7S_7$	1323.149862	0.610	-2	b8 - H2O, a8
1335.212899	21.4	$C_{46}H_{58}N_{12}O_{23}P_3S_3$	1335.212374	-0.390	-1	D4
1341.223974	31.9	$C_{46}H_{56}N_{16}O_{20}P_3S_3$	1341.223727	-0.180	-1	y4 - H2O, z4
1353.393705	68.1	$C_{172}H_{212}N_{56}O_{88}P_{15}S_{15}$	1353.393445	-0.190	-4	M - 5H
1353.645306	233.7	$C_{172}H_{213}N_{56}O_{88}P_{15}S_{15}$	1353.645264	-0.030	-4	M - 4H
1353.646583			1353.645264	-0.974	_	10
1365.791868	23.8	$C_{126}H_{157}N_{44}O_{66}P_{12}S_{12}$	1365.793265	1.020	-3	w12
1366.635676	38.0	$C_{86}H_{105}N_{30}O_{42}P_8S_8$	1366.634286	-1.020	-2	x8 - H2O
1367.127699	46.2	C ₈₆ H ₁₀₄ N ₂₉ O ₄₃ P ₈ S ₈	1367.126294	-1.030	-2	x8 - NH3
1370.127455	84.8	C ₈₄ H ₁₀₄ N ₃₀ O ₄₄ P ₈ S ₈	1370.125288	-1.580	-2	w8 - C2H4
1371.131351	37.5	C ₈₄ H ₁₀₆ N ₃₀ O ₄₄ P ₈ S ₈	1371.132839	1.090	-2	w8 - C2H2
1371.627848	20.4	$C_{86}H_{107}N_{26}O_{46}P_8S_8$	1371.625793	-1.500	-2	C8
1375.124564	48.1	$C_{131}H_{161}N_{38}O_{69}P_{12}S_{12}$	1375.125798	0.900	-3	a13 - B(A) - H2O, a13 - 5H
1378.614239	25.0	$C_{86}H_{105}N_{26}O_{47}P_8S_8$	1378.615151	0.660	-2	d8 - 5H
1384.141093	87.3	$C_{86}H_{108}N_{30}O_{44}P_8S_8$	1384.140939	-0.110	-2	w8
1395.129924	25.6	$C_{131}H_{163}N_{41}O_{70}P_{12}S_{12}$	1395.132394	1.770	-3	y13 - 4H
1431.158185	43.8	$C_{46}H_{59}N_{12}O_{25}P_4S_4$	1431.155861	-1.620	-1	d4
1455.179913	106.2	$C_{46}H_{59}N_{16}O_{23}P_4S_4$	1455.178328	-1.090	-1	w4
1556.655824	19.6	$C_{96}H_{120}N_{35}O_{49}P_9S_9$	1556.655777	-0.030	-2	w9
1557.157232	49.2	$C_{148}H_{178}O_{74}N_{51}P_{13}S_{13}$	1557.157113	-0.080	-3	z14 - 6H
1568.143761	19.2	C ₁₄₆ H ₁₈₂ O ₇₆ N ₄₈ P ₁₄ S ₁₄	1568.143026	-0.470	-3	c14 - OC2H2
1636.218643	40.5	$C_{56}H_{68}N_{14}O_{28}P_4S_4$	1636.217178	-0.900	-1	a5 - 2H
1637.224842	78.6	$C_{56}H_{69}N_{14}O_{28}P_4S_4$	1637.225003	0.100	-1	b5 - H2O, a5
1650.145239	27.2	$C_{51}H_{65}N_{15}O_{28}P_5S_5$	1650.142610	-1.590	-1	w5 - B(mC)
1805.192593	135.2	$C_{172}H_{214}N_{56}O_{88}P_{15}S_{15}$	1805.196111	1.950	-3	M - 3H
1805.192594	135.2	$C_{59}H_{74}N_{14}O_{32}P_5S_5$	1805.189620	-1.650	-1	a6 - B(T) - C2H2
1805.196082						
1812.187044	60.8	$C_{116}H_{140}N_{37}O_{59}P_{10}S_{10}$	1812.184592	-1.350	-2	a11 - NH2
1820.180831	70.8	$C_{61}H_{75}N_{11}O_{34}P_5S_5$	1820.178052	-1.530	-1	a6 - 3H
1821.189437	44.7	$C_{116}H_{142}N_{37}O_{60}P_{10}S_{10}$	1821.189600	0.090	-2	b11 - NH2
			Abs mean	0.679		
			error Abs mean std	0.532		
			dev	-		

Table S10 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-8H]⁸⁻ danvatirsen precursor ion by 2D-EDD-MS.

Measured	S/N	Elemental Theoretical		Error Charge Assignment			
mz		Composition	mz	(ppm)			
409.552864	51.3	$C_{29}H_{35}O_{15}N_5P_2S_2$	409.552864	0.000	-2	a3 - B(dA) - OC2H2	
598.806110	12.7	C ₇₄ H ₉₂ N ₂₅ O ₃₉ P ₇ S ₇	598.805499	-1.020	-4	w7 - OC2H2	
658.066901	30.7	C106H125N33O54P9S9	658.064150	-4.180	-5	a10 - 7H	
659,439887	74.3	C167H204N51O88P15S15	659.437182	-4.102	-8	M - 8H - A	
659,940365	223.3	$C_{22}H_{15}N_2P_5S_2$	659,940098	0.400	-		
662 272560	7.5	$C_{47}H_{22}N_{24}O_4S_2$	662 270605	2 950			
674 091208	15.8	$C_{00}H_{04}N_{00}O_{00}P_{5}S_{5}$	674 091053	-0.230	-3	v6	
675 200277	11.0	$C_{10}H_{17}O_{7}N_{17}P_{17}S_{17}$	675 198830	-2 140	-7	c14 - NH2	
677 605605	107.2	$CH_{a}N_{a}O_{a}O_{b}O_{a}O_{a}O_{a}O_{a}O_{a}O_{a}O_{a}O_{a$	677 603071	2 5/0	-1		
677 857350	15.0		677 857/33	0 110	-5	c10	
678 258016	10.0	$C_{106} = 1_{129} = 3_{33} = 0_{56} = 1_{10} = 0_{10}$	678 258007	0.110	-0	0.0	
691 2601/2	10.0		691 259001	3 010	Б	d10	
601.200142	20.4		601.230091	-3.010	-5	w10	
601 569004	20.1	$C \square N O D S$	601 566921	-2.720	-5	w8	
091.000994	0.0	$C_{86}\Pi_{106}N_{30}O_{44}P_8S_8$	091.000001	-3.130	-4		
092.008073	0.0	$C_{64}H_{80}N_{23}O_{33}P_6S_6$	092.008094	0.030	-3		
709.564247	18.3	$C_{91}H_{110}N_{26}O_{48}P_8S_8$	709.566360	2.980	-4	H2O, a9 - B(A)	
710.067257	48.5	$C_{111}H_{132}N_{40}O_{56}P_{10}S_{10}$	710.066542	-1.010	-5	y11 - 8H	
716.737698	14.3	$C_{136}H_{164}N_{46}O_{69}P_{12}S_{12}$	716.737851	0.210	-6	z13, y13 - H2O	
727.474935	33.2	$C_{116}H_{139}N_{38}O_{59}P_{10}S_{10}$	727.473216	-2.360	-5	a11, b11 - H2O	
743.329966	78.8	C ₉₆ H ₁₁₅ N ₃₁ O ₄₈ P ₈ S ₈	743.329984	0.020	-4	b9 - H2O, a9	
747.569034	29.9	$C_{51}H_{59}N_{10}O_{27}P_4S_4$	747.569771	0.990	-2	a5 - B(dC) - NH2	
751.641619	38.4	$C_{166}H_{202}N_{51}O_{88}P_{15}S_{15}$	751.640257	-1.810	-7	M - 7H - CH3 - A, M - 7H - CH3 - dA	
753.835147	13.4	$C_{96}H_{117}N_{35}O_{47}P_8S_8$	753.838241	4.100	-4	у9	
755.214411	40.6	$C_{167}H_{203}N_{53}O_{87}P_{15}S_{15}$	755.214409	0.000	-7	M - 7H - dC, M - 7H - mC	
766.753215	75.7	$C_{76}H_{92}N_{21}O_{39}P_6S_6$	766.754257	1.360	-3	a7, b7 - H2O	
772.935341	66.9	$C_{172}H_{209}N_{56}O_{88}P_{15}S_{15}$	772.935914	0.740	-7	M - 8H	
777.826157	24.3	C ₉₆ H ₁₁₈ N ₃₅ O ₄₉ P ₉ S ₉	777.824250	-2.450	-4	w9	
791.275195	21.9	$C_{126}H_{151}N_{40}O_{65}P_{11}S_{11}$	791.276180	1.240	-5	a12 - 6H	
796.882497	20.7	$C_{125}H_{151}N_{44}O_{64}P_{11}S_{11}$	796.879766	-3.430	-5	y12 - CH3	
809.410002	30.8	C ₁₅₃ H ₁₈₆ O ₈₀ N ₄₈ P ₁₄ S ₁₄	809.406947	-3.770	-6	a15 - B(dA) - OC2H2, a15 - B(dG) - C2H2, z15 - B(dA) - OC2H2, z15 - B(G) - C2H2	
812.747347	33.6	$C_{76}H_{95}N_{25}O_{40}P_7S_7$	812.746613	-0.900	-3	w7	
819.072246	196.5	$C_{126}H_{155}N_{44}O_{66}P_{12}S_{12}$	819.073048	0.980	-5	w12	
823.334659	38.0	C ₁₀₆ H ₁₂₈ N ₃₃ O ₅₄ P ₉ S ₉	823.335782	1.360	-4	a10, b10 - H2O	
824.086475	14.5	C ₁₀₅ H ₁₂₇ N ₃₃ O ₅₅ P ₉ S ₉	824.082692	-4.590	-4	b10 - CH3	
830.118236	26.1	$C_{56}H_{68}N_{18}O_{26}P_4S_4$	830.119822	1.910	-2	y5 - H2O, z5	
840,095692	29.8	$C_{10}H_{120}N_{40}O_{52}P_0S_0$	840.095661	-0.040	-4	y10	
860.285558	197.4	$C_{126}H_{165}N_{46}O_{60}P_{12}S_{12}$	860.286877	1.530	-5	z13, y13 - H2O	
881 764445	42.9	CeeH104N2eO44PzSz	881 764332	-0 130	-3	a8, b8 - H2O	
884 440009	64.9	$C_{00}H_{404}N_{20}O_{44}P_7S_7$	884 440000	-0.010	-3	v8 - H2O. z8	
902 094008	255 3	$C_{470}H_{044}N_{50}C_{411}$	902 09 <u>4</u> 417	0.450	-6	M - 6H	
Q15 8/5001	17 2	$C_{1/2}$ V_{211} V_{56} V_{88} V_{15} V_{15}	Q15 811050	-1 030	_4	v11 - NH3	
011 086170	1/ 5	C_{116} T_{139} 41058 10010	010.044009 011 027221		- - -	w11	
001 1100419	18.3	C_{116} 1_{143} 4_{2} C_{60} 1_{10} 1_{11}	001 110000	0.500		v9 - 0C2H2	
000 110060	10.0		000 440000	0.000	-5	V9 - H20 - 79	
333.449009	12.3	U96⊓ ₁₁₆ N35U46۲8S8	Abs mean	1.510	-3	yu - 1120, 29	

error Abs mea std dev	an 1.370
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Massured S/N Elemental Theoretic		Theoretical	Error	Charge	Assignment		
mz	5/N	Composition	mz	(nnm)	Charge	Assignment	
600 200905	20.7		600 200907	0.002			
009.300003	32.7	$C_{36}\Pi_{52}\Gamma_{3}S$	009.300007	0.003	0	o4 3⊔	
057.593534	19.1	$C_{46}\Pi_{54}N_{12}O_{22}P_3S_3$	007.093304	-0.270	-2	a4 - 511	
706.072033	8.9	$C_{66}H_{82}N_{23}O_{34}P_6S_6$	706.072032	0.000	-3	wo	
727.082478	10.6	$C_{46}H_{58}N_{16}O_{23}P_4S_4$	727.085251	3.810	-2	W4	
752.069594	6.7	$C_{141}H_{173}O_{74}N_{46}P_{13}S_{13}$	752.069657	0.080	-6	y14 - B(dA) -	
						B(T) - C2H2	
753 783044	88.9		753 786390	4 440	-7	M - 7H - dA, M -	
	00.0	0 167. 1203. 131 0 88. 130 13	1001100000			7H - A	
767.087703	7.4	$C_{51}H_{60}N_{15}O_{25}P_4S_4$	767.086728	-1.270	-2	z5 - 3H	
769.226156	5.7	C ₁₄₃ H ₁₇₃ O ₇₅ N ₄₆ P ₁₄ S ₁₄	769.226448	0.380	-6	c14 - 8H, x14 -	
						8H, x14 - B(dA)	
771 22/803	13.6	Current O Nu-PurSu	771 224443	-0 580	-6	- n20 x14 - B(mC) -	
111.224095	15.0	C143I 1171 O75I 147F 14O14	111.224445	-0.500	-0	NH2	
773.076333	1329.8	C ₁₄₆ H ₁₇₉ O ₇₆ N ₄₈ P ₁₃ S ₁₃	773.079889	4.600	-6	M - 7H	
775.094056	28.4	$C_{51}H_{62}N_{16}O_{25}P_4S_4$	775.095816	2.270	-2	y5 - 4H	
775.426043	14.8	$C_{76}H_{92}N_{24}O_{38}P_6S_6$	775.425876	-0.220	-3	y7 - NH2	
791.874770	9.5	$C_{125}H_{150}N_{40}O_{66}P_{11}S_{11}$	791.873708	-1.340	-5	b12 - CH4	
823.081745	8.3	$C_{106}H_{127}N_{22}O_{54}P_0S_0$	823.083826	2.530	-4	a10 - 5H	
857 909713	22.3	$C_{400}H_{400}O_{04}N_{50}P_{45}S_{45}$	857 910041	0.380	-6	w15, d15	
864 081054	23.0	C_{160} H_{196} C_{84} C_{53} H_{50} H_{400} N_{40} C_{53} P_{40} S_{40}	864 081532	0.550	_4	w10	
881 426771	74 5	$C_{100}H_{130}N_{20}O_{4}P_{7}S_{7}$	881 428208	1 630	-3	a8 - 4H	
881 583616	10.0	$C_{861} I_{1031} Q_{26} C_{441} 7 C_{7}$	881 583375	0.270	-5	z11 - 5H	
807 282440	13.0	$C_{111} I_{134} I_{37} O_{57} I_{10} O_{10}$	807 280727	1 020	-4 5	a14 - B(dA) -	
097.202449	11.1	C1411 173 C75 N43 F 13 C13	091.200121	-1.920	-5	C2H2	
901.927253	84.8	C172H210N56O88P15S15	901.926537	-0.790	-6	M - 7H	
905.590383	11.7	$C_{116}H_{138}N_{37}O_{56}P_{10}S_{10}$	905.588657	-1.910	-4	a11 - NH2	
909 596910	36.7	$C_{114}H_{140}N_{40}O_{57}P_{10}S_{10}$	909 598818	2 100	-4	y11 - OC2H2	
910 342717	38.6	C_{44} H 400 N 20 O 00 P 40 S 40	910 340111	-2 860	-4	, b11 - CH3	
922 426746	89.1	$C_{02}H_{407}N_{02}O_{44}P_{0}S_{0}$	922 424867	-2 040	-3	w8	
944 086516	12.2	$C_{440}H_{440}N_{40}O_{20}P_{44}S_{40}$	944 087331	0.860	_4	w11	
986 324995	13.7	C_{116} T_{143} T_{42} C_{60} T_{10}	986 324962	-0.030	-4 -4	w12 - B(A) -	
000.024000	10.7		000.024002	0.000	-	NH2, d12 - 5H	
989.598976	28.5	$C_{126}H_{153}N_{40}O_{65}P_{11}S_{11}$	989.599000	0.020	-4	b12 - H2O, a12	
991.442573	20.5	$C_{96}H_{116}N_{31}O_{48}P_8S_8$	991.442587	0.010	-3	b9 - H2O, a9	
995.600420	21.5	C ₁₂₆ H ₁₅₃ N ₄₄ O ₆₃ P ₁₁ S ₁₁	995.604617	4.220	-4	z12, y12 - H2O	
996.106329	21.3	C ₉₄ H ₁₁₄ N ₃₅ O ₄₇ P ₈ S ₈	996.109647	3.330	-3	y9 - C2H4	
1024.091555	75.4	C ₁₂₆ H ₁₅₆ N ₄₄ O ₆₆ P ₁₂ S ₁₂	1024.093130	1.540	-4	w12	
1037.434604	29.0	$C_{96}H_{119}N_{35}O_{49}P_9S_9$	1037.434577	-0.030	-3	w9	
1052.504799	19.8	C ₁₆₇ H ₂₀₇ N ₅₁ O ₈₇ P ₁₅ S ₁₅	1052.504874	0.070	-5	M - 5H - G, M -	
					_	5H - dG	
1059.613228	9.9	$C_{66}H_{83}N_{23}O_{34}P_6S_6$	1059.611961	-1.200	-2	W6	
1066.083472	13.2	$C_{129}H_{161}N_{44}O_{70}P_{13}S_{13}$	1066.084284	0.760	-4	w13 - B(T) -	
1069 611823	11 2	Cuarthan Nuo One Pue Suo	1069 610552	_1 100	_4	v13 - OC2H2	
1075 608471	38.5	C_{134} Γ_{166} Γ_{46} C_{69} Γ_{12} C_{12}	1075 610415	1 810	-4	v13 - H2O, z13	
1073.000471	35.7	C = N = O = S	1073.010413	1.620	-4	M - 7H	
1115 454022	24 5	C = 172112101156088F15015	1115 /55/91	0.400	-5	v10 - CH3	
1010 600000	24.5	$C_{105} I_{127} I_{40} O_{52} F_{9} O_{9}$	1010 600004	0.490	-3	w7	
1219.022902	17.4	$C_{76}\Pi_{96}\Pi_{25}O_{40}P_7S_7$	1219.023204	0.200	-2	W7 M ALL 2T	
1259.113350	11.0	$C_{157}H_{195}N_{50}O_{82}P_{15}O_{15}$	1209.113200	-0.120	-4	WO	
1000.000498	10.3	U ₉₆ ⊓ ₁₂₀ N ₃₅ U ₄₉ P ₉ S ₉	1000.000003	0.000	-2	vv 3	
			Abs mean	1.324			
			error	4 007			
			Abs mean	1.207			
			std dev				

Table S11 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-7H]⁷⁻ danvatirsen precursor ion by 2D-EDD-MS.

Measured	S/N	Flemental	Theoretical	Frror	Charge	Assignment
mz	0/11	Composition	mz	(ppm)	onarge	Assignment
773 228418	13.0	C142H171O74N40P14S14	773 226315	-2 720	-6	x14 - 9H
782.649897	12.4	$C_{120}H_{143}N_{37}O_{66}P_{12}S_{12}$	782.649965	0.090	-5	c12 - B(dC) -
					-	CH4
817.605421	12.1	$C_{56}H_{67}N_{14}O_{28}P_4S_4$	817.604950	-0.580	-2	a5 - 3H
876.913662	13.5	$C_{166}H_{202}N_{51}O_{88}P_{15}S_{15}$	876.913542	-0.140	-6	M - 6H - CH4 - A M - 6H - CH4
						- dA
877.080841	16.5	$C_{111}H_{132}N_{37}O_{56}P_{10}S_{10}$	877.080734	-0.120	-4	z11 - 7H
877.579937	12.4	$C_{111}H_{132}N_{36}O_{57}P_{10}S_{10}$	877.578694	-1.420	-4	z11 - B(A) -
880 078501	23.2		880 077500	-1.030	_1	711 - B(mC) -
000.070001	20.2		000.011000	1.000	т	NH3
880.410501	12.3	C ₈₁ H ₁₀₁ N ₂₈ O ₄₂ P ₈ S ₈	880.410558	0.060	-3	w8 - B(T)
887.095694	26.9	$C_{86}H_{104}N_{26}O_{45}P_7S_7$	887.095788	0.110	-3	b8 - 5H
899.424283	17.5	C ₁₇₂ H ₂₀₉ N ₅₅ O ₈₈ P ₁₅ S ₁₅	899.424630	0.390	-6	M - 6H - NH2
899.591417	33.9	$C_{171}H_{208}N_{56}O_{88}P_{15}S_{15}$	899.590596	-0.910	-6	M - 6H - CH3
901.087073	13.9	$C_{59}H_{71}N_{14}O_{32}P_5S_5$	901.083346	-4.140	-2	аб - В(Т) - С2Н4
901.276073	7.5	$C_{142}H_{169}O_{74}N_{45}P_{13}S_{13}$	901.276603	0.590	-5	a14 - B(mC) -
004 476674	110		001 470460	1 660	F	CH4
901.476671	14.2	$C_{142}\Pi_{170}O_{74}\Pi_{45}P_{13}O_{13}$	901.478108	1.000	-5	CH3
902.568150	145.7	$C_{111}H_{135}N_{35}O_{60}P_{11}S_{11}$	902.566438	-1.900	-4	d11 - B(T) -
						NH2, c11 - B(dC)
902.587107	3375.9	C114H136N38O59P10S10	902.585513	-1.770	-4	a11 - C2H4
902.753808	2819.6	$C_{84}H_{104}N_{30}O_{42}P_8S_8$	902.753766	-0.050	-3	x8 - OC2H2
903.087350	1280.0	C ₁₁₄ H ₁₃₈ N ₃₈ O ₅₉ P ₁₀ S ₁₀	903.089289	2.150	-4	a11 - C2H2
903.587386	188.2	$C_{59}H_{74}N_{13}O_{33}P_5S_5$	903.590730	3.700	-2	b6 - B(dC) -
904 087315	15 3		904 084605	-3 000	-5	0C2H2 a14 - 6H. z14 -
304.007313	10.0	01431 1173 0731 461 13013	304.004003	-0.000	-0	6H
906.084658	166.8	C ₁₄₃ H ₁₇₁ O ₇₂ N ₄₈ P ₁₃ S ₁₃	906.083722	-1.030	-5	z14 - B(T) - NH2
906.583893	73.7	C ₆₁ H ₇₂ N ₁₃ O ₃₂ P ₅ S ₅	906.585448	1.720	-2	a6 - B(dC) -
						H2O, a6 - B(T)
909 082939	38 1		909 081475	-1 610	-2	a6 - 5H
909.587429	13.2	$C_{61}H_{74}N_{11}O_{34}P_5S_5$	909.585387	-2.240	-2	a6 - 4H
912.082526	6.8	$C_{60}H_{75}N_{11}O_{35}P_5S_5$	912.086483	4.340	-2	b6 - B(dA) -
000 404404	17.0		000 404604	0 5 2 0	2	CH3
922.424191	17.9	$C_{86}\Pi_{107}N_{30}O_{44}P_8S_8$	922.424084	0.530	-3	wo 26 - 3H
977.014020	20.0	$C_{66}\Pi_{80}N_{16}O_{34}P_5O_5$	9/1.0102/4	2.300	-2	a0 - 511 b6 - NH3
970.010772	30.Z 12.5	$C_{66} \Pi_{80} N_{15} O_{35} \Gamma_5 O_5$	970.012400	-4.400	-2	b12 - NH3
1000 1117/0	12.0	$C_{1261} = 1521 \times 390661 = 11011$	1000 100830	-0.230		v9 - CH4
1024 090111	14.7	$C_{95}H_{114}N_{35}O_{47}H_{8}O_{8}$	1024 087696	-2.360	-3	d9 - NH2
1024.589666	31.6	$C_{120}H_{158}N_{38}O_{60}P_{12}S_{12}$	1024.588754	-0.890	-4	a13 - B(G) -
1000 005500	04.0		1000 000 100	0.040	-	C2H4
1029.685528	24.8	$C_{161}H_{195}N_{50}O_{86}P_{15}S_{15}$	1029.686496	0.940	-5	2dC
1031.091806	16.4	$C_{131}H_{160}N_{38}O_{69}P_{12}S_{12}$	1031.092530	0.700	-4	a13 - 6H, a13 - B(A) - H2O
1038.094524	57.1	$C_{131}H_{160}N_{40}O_{69}P_{12}S_{12}$	1038.094204	-0.310	-4	a13 - B(mC),
						b13 - B(mC) -
						п20, b13 - b(1) - NH3
1059.609903	25.6	C ₆₆ H ₈₃ N ₂₃ O ₃₄ P ₆ S ₆	1059.611687	1.680	-2	w6
1076.604313	22.3	C ₇₀ H ₈₇ N ₁₆ O ₃₉ P ₆ S ₆	1076.604138	-0.160	-2	b7 - B(G) - CH3
1083.075702	11.9	$C_{100}H_{121}N_{31}O_{54}P_{10}S_{10}$	1083.075830	0.120	-3	c10 - B(T) -
1083 105705	218.0		1083 107777	1 820	_2	CH4 b7-4H a7-
1003.103793	210.9	0711 1881 16 039 F 606	1005.107777	1.000	-2	B(dA), b7 -

Table S12 showing peak list, signal-to-noise ratio (S/N), elemental composition, and possible assignments with mass errors (ppm) of the [M-6H]⁶⁻ danvatirsen precursor ion by 2D-EDD-MS.

1098.110131 1098.444620 1098.776345 1151.130421 1151.630570 1153.433485	27.4 16.9 25.7 11.3 12.5 36.1	$\begin{array}{c} C_{71}H_{84}N_{23}O_{35}P_6S_6\\ C_{106}H_{128}N_{32}O_{55}P_9S_9\\ C_{105}H_{127}N_{33}O_{55}P_9S_9\\ C_{76}H_{92}N_{20}O_{40}P_6S_6\\ C_{76}H_{93}N_{20}O_{40}P_6S_6\\ C_{109}H_{132}N_{33}O_{58}P_{10}S_{10}\\ \end{array}$	1098.113057 1098.444807 1098.776557 1151.127306 1151.630945 1153.433307	2.660 0.170 0.190 -2.710 0.330 -0.150	-2 -3 -3 -2 -2 -3	B(dA) - H2O z7 - 5H b10 - NH3 b10 - CH4 b7 - NH3 b7 - NH2 a11 - B(G) - C2H4 a15 - B(dG) -
1214.115839 1259.106145 1260.104192	12.4 21.1 30.1	C ₁₅₃ H ₁₈₆ O ₈₀ N ₄₈ P ₁₄ S ₁₄ C ₈₁ H ₉₅ N ₂₃ O ₄₃ P ₇ S ₇ C ₁₁₉ H ₁₄₅ N ₃₅ O ₆₄ P ₁₁ S ₁₁	1259.108669 1260.107522	-4.690 2.000 2.640	-4 -2 -3	a 15 - 6(06) - C2H4, z15 - B(G) - C2H4 a8 - 5H a12 - B(G) - C2H4
1329.108128 1354.116802 1554.823124	10.4 39.3 9.4	$\begin{array}{c} C_{41}H_{51}N_{13}O_{22}P_4S_4\\ C_{126}H_{154}N_{44}O_{64}P_{12}S_{12}\\ C_{146}H_{179}O_{75}N_{51}P_{13}S_{13} \end{array}$	1329.111043 1354.122164 1554.824509 Abs mean error Abs mean std dev	2.190 3.960 0.890 1.649 1.238	-1 -3 -3	w4 - 2H x12 - H2O y14 - C2H4

Table S13 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of one scan denoised (sane rank 10) [M-8H]⁸⁻ precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured	Intensity	Elemental	Theoretical	Error	Charg	Assignmen
mz	-	Composition	mz	(ppm	е	t
)		
225.560984	1740907.0					
225.564220	2472008.7					
338.157749	13274609.6					
338.167652	1797371.3					
338.210996	4110571.8					
338.220422	29988344.8					
338.229929	4303612.9					
338.274284	3284753.3					
338.283048	33029211.8					
338.292211	4172903.8					
338.344567	7808075.3					
338.400417	2226435.6					
338.408269	14765760.8					
338.416373	2010386.8					
338.462275	1705712.6					
338.470583	22471378.7					
338.478993	1819578.4					
338.533041	18285322.3					
338.543014	2596628.7					
338.595163	7180541.1					
338.657361	2040699.1					
338.658672	1770008.4					
338.720658	1827530.5					
339.866196	2043140.2					
541.254272	2122260.4					
601.395200	3262256.6					
609.308001	3269107.6	$C_{76}H_{98}N_{25}O_{40}P_7S_7$	609.308004	0.005	-4	w7
657.563909	2050827.9					
657.593028	3516477.7					
659.438177	3118306.4					
659.565777	4440149.1					
659.689513	11226883.5					
659.815492	10058763.5					
659.938761	4761343.7					
673.823356	1858546.2					
673.948559	1788057.1					
674.072977	2127635.3					
674.091895	4450368.8	$C_{66}H_{84}N_{23}O_{32}P_5S_5$	674.090870	-	-3	у6
				1.521		
674.323228	17057623.6					
674.448454	37431606.0					
674.535295	2237489.1					
674.547643	1847308.9					
674.573701	56003409.2					
674.659884	2463284.7					
674.698669	68020902.2					
674.722873	2284603.4					
674.735919	1879203.5					
674.784842	2426621.4					
674.799736	2130285.2					

	674.823907	61461539.8						
	674.909703	2818066.0						
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	674.924147	2034247.5						
$ \begin{array}{l} 675.073537 & 30691037.1 \\ 675.19837 & 225442116 \\ 675.323175 & 13207262.5 \\ 675.573847751 & 9029169.8 \\ 675.573842 & 4935024.4 \\ 675.673824 & 4935024.4 \\ 676.078851 & 2806215.3 \\ 676.078851 & 2806215.3 \\ 676.078851 & 2008056.5 \\ 676.118543 & 2144552.7 \\ 676.113543 & 2144552.7 \\ 676.113543 & 2144559.3 \\ 676.1412 & 212937.5 \\ 676.153333 & 178000.6 \\ 676.172063 & 2537847.0 \\ 676.172063 & 2537847.0 \\ 676.172063 & 2537847.0 \\ 676.172063 & 2537847.0 \\ 676.172063 & 2537847.0 \\ 676.20586 & 4392098.2 \\ 676.2217123 & 3406627.8 \\ 676.22524 & 6424758.7 \\ 676.26252 & 5780503.6 \\ 676.225274 & 6424758.7 \\ 676.26252 & 5780503.6 \\ 676.295290 & 18312119.5 \\ 676.320085 & 580758939.5 \\ C_{112}H_{217}N_{56}O_{88}P_{16}S & 676.318994 & 1.613 & -8 \\ 15 \\ 676.34300 & 22219809.5 \\ 676.34300 & 22219809.5 \\ 676.341303 & 16823494.2 \\ 676.341332 & 15371881.0 \\ 676.449048 & 62122979.4 \\ 676.449342 & 239978.7 \\ 676.449342 & 239978.7 \\ 676.449342 & 239978.7 \\ 676.449340 & 23991641.2 \\ 676.448551 & 37018959.8 \\ 676.496340 & 23991641.2 \\ 676.591682 & 77138646.0 \\ 676.692465 & 582741.9 \\ 676.619805 & 35327541.9 \\ 676.624565 & 378032744.9 \\ 11347726.1 \\ 776.628566 & 337449.1 \\ 676.632633 & 11341706.7 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.674853 & 77738646.0 \\ 676.6784552 & 777138646.0 \\ 676.6784552 & 777138646.0 \\ 676.674927 & 935327541.9 \\ 676.6784558 & 677557074 \\ 211137752.0 \\ 676.6784558 & 677557074 \\ 211137752.0 \\ 676.6784558 & 677557074 \\ 211137752.0 \\ 676.6784558 & 677557074 \\ 211137752.0 \\ 676.6784558 & 677557074 \\ 211137752.0 \\ 676.6784558 & 677557074 \\ 211137752.0 \\ 676.6784558 & 677557074 \\ 211137752.0 \\ 676.6784558 & 677557074 \\ 77738646.0 \\ 676.6784558 & 677557744558 \\ 77738646.0 \\ 776.6784558 & 67755774 \\ 77738646.0 \\ 77738646$	674.948773	49187437.3						
$ \begin{array}{c} 675.198378 & 22544211.6 \\ 675.323175 & 13207262.5 \\ 675.447751 & 9029169.8 \\ 675.573842 & 4935024.4 \\ 676.078851 & 2806215.3 \\ 676.065599 & 2180528.4 \\ 676.078851 & 2806215.3 \\ 676.10736 & 2080056.5 \\ 676.118543 & 2144857.7 \\ 676.13562 & 2144459.3 \\ 676.16322 & 2144859.3 \\ 676.16322 & 2144859.3 \\ 676.16322 & 2144859.3 \\ 676.16327 & 234400.6 \\ 676.16327 & 234400.2 \\ 676.1819 & 2301547.2 \\ 676.205386 & 4392098.2 \\ 676.21719 & 9640054.7 \\ 676.235204 & 5127274.1 \\ 676.205386 & 4392098.2 \\ 676.27199 & 9640054.7 \\ 676.282903 & 20794313.8 \\ 676.282903 & 20794313.8 \\ 676.295290 & 18312119.5 \\ 676.361034 & 16823494.2 \\ 676.378127 & 14278468.8 \\ 676.378127 & 14278468.8 \\ 676.378127 & 14278468.8 \\ 676.445526 & 1339304528. \\ 0 \\ 676.445526 & 1339304528. \\ 0 \\ 676.468426 & 50599789.7 \\ 676.479270 & 30373811.2 \\ 676.479270 & 30373811.2 \\ 676.479270 & 30373811.2 \\ 676.468426 & 50599789.7 \\ 676.468426 & 50599789.7 \\ 676.468426 & 50599789.7 \\ 676.479270 & 30373811.2 \\ 676.54630 & 229218858.8 \\ 676.496340 & 23991641.2 \\ 676.5132633 & 111341706.7 \\ 676.591682 & 77138646.0 \\ 676.62455 & 83718934.0 \\ 0 \\ 776.54360 & 6624455.8 \\ 676.670704 & 2111879384. \\ 0 \\ 776.543660 & 6624455.8 \\ 676.63133 & 37636107.8 \\ 676.63133 & 37636107.8 \\ 676.63133 & 37636107.8 \\ 676.637391 & 134932471.9 \\ 676.695805 & 2350566485. \\ 0 \\ 0 \\ 676.712388 & 98535232.1 \\ \end{array}$	675.073537	30691037.1						
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	675.198378	22544211.6						
$\begin{array}{c} 675.447751 & 9029169.8 \\ 675.573842 & 4935024.4 \\ 676.078559 & 2450861.8 \\ 676.078551 & 2806215.3 \\ 676.0736 & 2086056.5 \\ 676.118543 & 2148572.7 \\ 676.13532 & 2144589.3 \\ 676.118532 & 2144589.3 \\ 676.153323 & 2144589.3 \\ 676.153323 & 2144589.3 \\ 676.153323 & 2144589.3 \\ 676.16327 & 2344002.6 \\ 676.163327 & 2344002.6 \\ 676.163327 & 2344002.6 \\ 676.172063 & 2537847.0 \\ 676.205386 & 4392098.2 \\ 676.221742 & 3589781.0 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.320025 & 580758939.5 \\ C_{172}H_{217}N_{58}O_{80}P_{15}S & 676.318994 & 1.613 & -8 \\ \end{array}$	675.323175	13207262.5						
$ \begin{array}{c} 675.577.842 & 4935024.4 \\ 675.692539 & 2450861.8 \\ 676.076859 & 2180528.4 \\ 676.078851 & 2806215.3 \\ 676.10736 & 2088056.5 \\ 676.118543 & 2144572.7 \\ 676.135623 & 2144589.3 \\ 676.14512 & 2129377.5 \\ 676.153393 & 1780000.6 \\ 676.163327 & 2344002.6 \\ 676.172063 & 2537847.0 \\ 676.172063 & 2537847.0 \\ 676.217123 & 3406627.8 \\ 676.223742 & 3406627.8 \\ 676.22524 & 5127274.1 \\ 676.252274 & 6424758.7 \\ 676.252274 & 6424758.7 \\ 676.252274 & 6424758.7 \\ 676.25228 & 5780503.6 \\ 676.22702 & 5127274.1 \\ 676.25228 & 5780503.6 \\ 676.22903 & 20794313.8 \\ 676.282903 & 20794313.8 \\ 676.282903 & 20794313.8 \\ 676.320085 & 580758939.5 \\ C_{172}H_{217}N_{56}O_{38}P_{15}S & 676.318994 & 1.613 & -8 \\ 15 \\ 676.361034 & 16823494.2 \\ 676.361034 & 16823494.2 \\ 676.381432 & 15371881.0 \\ 676.448642 & 50599789.7 \\ 676.445526 & 1339304528. \\ 0 \\ 676.445526 & 1339304528. \\ 0 \\ 676.4468426 & 50599789.7 \\ 676.445526 & 1339304528. \\ 0 \\ 676.4468426 & 50599789.7 \\ 676.445526 & 1339304528. \\ 0 \\ 676.496340 & 23991641.2 \\ 676.496340 & 23991641.2 \\ 676.591682 & 77138646.0 \\ 676.532033 & 11341706.7 \\ 676.54315 & 27669320.6 \\ 676.532033 & 11341706.7 \\ 676.54315 & 27569320.6 \\ 676.570704 & 2111879384. \\ 0 \\ 676.695806 & 8244585.8 \\ 676.631425 & 5807752.0 \\ 676.619805 & 33651643.8 \\ 676.631425 & 5807744.1 \\ 676.649854 & 37018959.8 \\ 676.619805 & 33651643.8 \\ 676.632128 & 77138646.0 \\ 676.632128 & 77138646.0 \\ 676.632128 & 77138646.0 \\ 676.67822 & 78057744.1 \\ 676.695805 & 33651643.8 \\ 676.632282 & 78057744.1 \\ 676.695805 & 336566485. \\ 0 \\ 0 \\ 676.712388 & 98535232.1 \\ \end{array}$	675 447751	9029169.8						
$\begin{array}{c} 153024 \\ 755.692539 & 2450261.8 \\ 7676.07851 & 2006215.3 \\ 7676.073651 & 2006215.3 \\ 7676.135623 & 2144589.3 \\ 7676.135623 & 2144589.3 \\ 7676.135623 & 2144589.3 \\ 7676.135623 & 2144589.3 \\ 7676.15012 & 2129377.5 \\ 7676.15393 & 1780000.6 \\ 7676.16199 & 2001547.2 \\ 7676.12053 & 2537847.0 \\ 7676.1199 & 2001547.2 \\ 7676.205386 & 4392098.2 \\ 7676.22374 & 5242758.7 \\ 7676.225274 & 6242758.7 \\ 7676.225274 & 6242758.7 \\ 7676.225200 & 18312119.5 \\ 7676.235204 & 5127274.1 \\ 7676.235204 & 5127274.1 \\ 7676.235200 & 20794313.8 \\ 7676.295290 & 18312119.5 \\ 7676.320085 & 580758939.5 \\ C_{172}H_{217}N_{56}O_{80}P_{15}S & 676.318994 & 1.613 & -8 \\ \end{array}$	675 573842	4935024 4						
$\begin{array}{c} 675.05599 & 2180528.4 \\ 676.078851 & 2805215.3 \\ 676.10736 & 2088056.5 \\ 676.118543 & 2148572.7 \\ 676.135623 & 2144589.3 \\ 676.14512 & 212937.5 \\ 676.153393 & 1780000.6 \\ 676.153393 & 1780000.6 \\ 676.163327 & 2344002.6 \\ 676.172063 & 2537847.0 \\ 676.172063 & 2537847.0 \\ 676.2172063 & 2537847.0 \\ 676.223742 & 3589781.0 \\ 676.223742 & 3589781.0 \\ 676.223742 & 3589781.0 \\ 676.223742 & 5127274.1 \\ 676.252274 & 6424758.7 \\ 676.223749 & 9640654.7 \\ 676.223749 & 9640654.7 \\ 676.223920 & 18312119.5 \\ 676.230085 & 580758939.5 \\ 676.260528 & 5780533.6 \\ 676.27149 & 9640654.7 \\ 676.242903 & 20794313.8 \\ 676.295290 & 18312119.5 \\ 676.30085 & 580758939.5 \\ 676.361034 & 16823494.2 \\ 676.378127 & 14278468.8 \\ 676.34332 & 15371881.0 \\ 676.408048 & 62122979.4 \\ 676.419374 & 45851471.6 \\ 676.445526 & 1339304528. \\ 0 \\ 676.46515 & 37018959.8 \\ 676.496340 & 23991641.2 \\ 676.445526 & 1339304528. \\ 0 \\ 676.46553 & 11134706.7 \\ 676.436515 & 37018959.8 \\ 676.496340 & 23991641.2 \\ 676.54360 & 66244585.8 \\ 676.570704 & 2111879384. \\ 0 \\ 676.591682 & 77138646.0 \\ 676.638135 & 37636107.8 \\ 676.61245 & 56017752.0 \\ 676.619805 & 35327541.9 \\ 676.67391 & 34932471.9 \\ 676.67822 & 78977449.1 \\ 676.6657391 & 134932471.9 \\ 676.67282 & 78077449.1 \\ 676.657391 & 34932471.9 \\ 676.6712386 & 98535232.1 \\ \end{array}$	675 692539	2450861.8						
$\begin{array}{c} 0.1000303 \\ 0.1000305 \\ 0.100036 \\ 0.100036 \\ 0.100036 \\ 0.100036 \\ 0.100036 \\ 0.100036 \\ 0.100036 \\ 0.100036 \\ 0.10036$	676 065500	2180528 /						
$\begin{array}{c} 0100000000000000000000000000000000000$	676 07005399	2100320.4						
$\begin{array}{c} 0.100736\\ 0.100736\\ 0.145012\\ 0.145012\\ 0.145012\\ 0.145012\\ 0.145012\\ 0.145012\\ 0.145012\\ 0.145012\\ 0.145012\\ 0.14502\\ 0.1$	676 100726	2000210.0						
$\begin{array}{c} 0 \text{ for } 116943 & 2146972.7 \\ 0 \text{ for } 116943 & 2144589.3 \\ 0 \text{ for } 163327 & 2344002.6 \\ 0 \text{ for } 153327 & 2344002.6 \\ 0 \text{ for } 1613327 & 2344002.6 \\ 0 \text{ for } 12003 & 2537847.0 \\ 0 \text{ for } 1219 & 2301547.2 \\ 0 \text{ for } 2537847.0 \\ 0 \text{ for } 2537847.0 \\ 0 \text{ for } 253724 & 3589781.0 \\ 0 \text{ for } 25274 & 0424758.7 \\ 0 \text{ for } 252274 & 0424758.7 \\ 0 \text{ for } 25228 & 5780503.6 \\ 0 \text{ for } 252290 & 18312119.5 \\ 0 \text{ for } 320085 & 580758939.5 \\ 0 \text{ for } 32085 & 580758939.5 \\ 0 \text{ for } 344300 & 22219809.5 \\ 0 \text{ for } 344320 & 22219809.5 \\ 0 \text{ for } 344321 & 15371881.0 \\ 0 \text{ for } 344322 & 15371881.0 \\ 0 \text{ for } 344322 & 15371881.0 \\ 0 \text{ for } 408048 & 62122979.4 \\ 0 \text{ for } 646340 & 23991641.2 \\ 0 \text{ for } 6468426 & 50599789.7 \\ 0 \text{ for } 646340 & 23991641.2 \\ 0 \text{ for } 65222 & 28265522.1 \\ 0 \text{ for } 6514315 & 27569320.6 \\ 0 \text{ for } 652453 & 3111341706.7 \\ 0 \text{ for } 652453 & 3111341706.7 \\ 0 \text{ for } 652453 & 311341706.7 \\ 0 \text{ for } 676.543660 & 66244585.8 \\ 0 \text{ for } 6526582 & 1111879384. \\ 0 \text{ for } 676.638135 & 37636107.8 \\ 0 \text{ for } 676.638135 & 37636107.8 \\ 0 \text{ for } 676.63825 & 7807449.1 \\ 0 \text{ for } 677.12388 & 98535232.1 \\ \end{array}$	070.100730	2000030.3						
$\begin{array}{c} 0 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ $	070.110043	2148572.7						
	676.135623	2144589.3						
	676.145012	2129377.5						
$\begin{array}{c} 676.173327\\ 2344002.6\\ 676.17206\\ 2576.17123\\ 4392098.2\\ 676.27123\\ 4392098.2\\ 676.271723\\ 4392098.2\\ 676.235204\\ 5127274.1\\ 676.235204\\ 5127274.1\\ 676.235204\\ 5127274.1\\ 676.235204\\ 5127274.1\\ 676.25227\\ 6424758.7\\ 676.25220\\ 18312119.5\\ 676.230085\\ 580758939.5\\ C_{172}H_{217}N_{56}O_{80}P_{15}S\\ 676.318994\\ 1.613\\ -8\\ 676.344300\\ 22219809.5\\ 676.361034\\ 16823494.2\\ 676.378127\\ 14278468.8\\ 676.344302\\ 22219809.5\\ 676.361034\\ 16823494.2\\ 676.378127\\ 14278468.8\\ 676.344322\\ 15371881.0\\ 676.44526\\ 1339304528.\\ 0\\ 676.445526\\ 1339304528.\\ 0\\ 676.445526\\ 30373811.2\\ 676.468426\\ 50599789.7\\ 676.479270\\ 30373811.2\\ 676.468426\\ 50599789.7\\ 676.479270\\ 30373811.2\\ 676.468456\\ 1339304528.\\ 0\\ 676.55292\\ 28265522.1\\ 676.514315\\ 27569320.6\\ 676.55292\\ 28265522.1\\ 676.514315\\ 27569320.6\\ 676.53606\\ 6244585.8\\ 676.570704\\ 2111879384.\\ 0\\ 0\\ 676.691245\\ 38581643.8\\ 676.611245\\ 56017752.0\\ 676.638135\\ 3763817.8\\ 0\\ 676.63823\\ 7837541.9\\ 0\\ 676.63822\\ 78977449.1\\ 676.69586\\ 2350566485.\\ 0\\ 0\\ 676.67822\\ 78977449.1\\ 676.695805\\ 2350566485.\\ 0\\ 0\\ 676.712388\\ 98535232.1\\ \end{array}$	676.153393	1780000.6						
$\begin{array}{c} 676.172063 \\ 2301547.2 \\ 676.205386 \\ 4392098.2 \\ 676.217123 \\ 3406627.8 \\ 676.223742 \\ 5389781.0 \\ 676.235204 \\ 5127274.1 \\ 676.26528 \\ 5780503.6 \\ 676.271499 \\ 9646054.7 \\ 676.282903 \\ 20794313.8 \\ 676.282903 \\ 20794313.8 \\ 676.295290 \\ 18312119.5 \\ 676.320085 \\ 580758939.5 \\ C_{172}H_{217}N_{56}O_{89}P_{15}S \\ 676.318994 \\ 1.613 \\ -8 \\ \end{array}$	676.163327	2344002.6						
$\begin{array}{c} 676.181199 & 2301547.2 \\ 676.205386 & 4392098.2 \\ 676.217123 & 3406627.8 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.235204 & 5127274.1 \\ 676.26528 & 5780503.6 \\ 676.271499 & 9646054.7 \\ 676.282903 & 20794313.8 \\ 676.282903 & 20794313.8 \\ 676.282903 & 20794313.8 \\ 676.282903 & 20794313.8 \\ 676.382085 & 580758939.5 \\ 676.320085 & 580758939.5 \\ 676.344300 & 22219809.5 \\ 676.344300 & 22219809.5 \\ 676.38127 & 14278468.8 \\ 676.38432 & 15371881.0 \\ 676.44932 & 15371881.0 \\ 676.449526 & 1339304528. \\ 0 \\ 676.468426 & 50599789.7 \\ 676.479270 & 30373811.2 \\ 676.46515 & 37018959.8 \\ 676.496340 & 23991641.2 \\ 676.514315 & 27569320.6 \\ 676.55292 & 28265522.1 \\ 676.514315 & 27569320.6 \\ 676.55263 & 111341706.7 \\ 676.543600 & 66244585.8 \\ 676.670704 & 2111879384. \\ 0 \\ 0 \\ 676.619805 & 35327541.9 \\ 676.628265 & 77138646.0 \\ 676.628265 & 38745838.0 \\ 676.638135 & 376636107.8 \\ 676.638135 & 376636107.8 \\ 676.675791 & 134932471.9 \\ 676.678822 & 78977449.1 \\ 676.69805 & 2350566485. \\ 0 \\ 0 \\ 676.712388 & 98535232.1 \\ \end{array}$	676.172063	2537847.0						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.181199	2301547.2						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.205386	4392098.2						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.217123	3406627.8						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.223742	3589781.0						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.235204	5127274.1						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.252274	6424758.7						
$\begin{array}{c} 676.271499 & 9646054.7 \\ 676.282903 & 20794313.8 \\ 676.295290 & 18312119.5 \\ 676.320085 & 580758939.5 & C_{172}H_{217}N_{56}O_{88}P_{15}S & 676.318994 & 1.613 & -8 \\ \end{array}$	676.260528	5780503.6						
$\begin{array}{c} 676.282903 \\ 676.282903 \\ 20794313.8 \\ 676.295290 \\ 18312119.5 \\ 676.320085 \\ 580758939.5 \\ C_{172}H_{217}N_{56}O_{88}P_{15}S \\ 676.318994 \\ 1.613 \\ -8 \\ \end{array}$	676 271499	9646054 7						
$\begin{array}{c} 676.29529 \\ 676.320085 \\ 580758939.5 \\ C_{172}H_{217}N_{56}O_{38}P_{15}S \\ 676.318994 \\ 1.613 \\ -8 \\ \end{array}$	676 282903	20794313 8						
$\begin{array}{c} 676.320085 & 580758939.5 & C_{172}H_{217}N_{56}O_{88}P_{15}S & 676.318994 & 1.613 & -8 \\ \end{array} \\ \begin{array}{c} 676.344300 & 22219809.5 \\ 676.361034 & 16823494.2 \\ 676.378127 & 14278468.8 \\ 676.378127 & 14278468.8 \\ 676.498048 & 62122979.4 \\ 676.419374 & 45851471.6 \\ 676.445526 & 1339304528. \\ 0 \\ \end{array} \\ \begin{array}{c} 676.468426 & 50599789.7 \\ 676.479270 & 30373811.2 \\ 676.496340 & 23991641.2 \\ 676.505292 & 28265522.1 \\ 676.505292 & 28265522.1 \\ 676.514315 & 27569320.6 \\ 676.532633 & 111341706.7 \\ 676.543660 & 66244585.8 \\ 676.570704 & 2111879384. \\ 0 \\ \end{array} \\ \begin{array}{c} 676.6591682 & 77138646.0 \\ 676.611245 & 56017752.0 \\ 676.619805 & 35327541.9 \\ 676.629566 & 38745838.0 \\ 676.678822 & 78977449.1 \\ 676.678822 & 78977449.1 \\ 676.695805 & 2350566485. \\ 0 \\ \end{array} $	676 295290	18312119.5						
$\begin{array}{c} 15\\ 676.324300\\ 22219809.5\\ 676.361034\\ 16823494.2\\ 676.378127\\ 14278468.8\\ 676.378127\\ 14278468.8\\ 676.384332\\ 15371881.0\\ 676.408048\\ 62122979.4\\ 676.419374\\ 45851471.6\\ 676.445526\\ 1339304528.\\$	676 320085	580758939 5		PS	676 318004	1 613	-8	M - 8H
	010.020000	000100000.0	01/21 121/1 056 088	150	070.010004	1.010	0	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676 344300	22210800 5	15					
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676 261024	16022404.2						
$\begin{array}{c} 676.376127 & 14276406.6 \\ 676.384332 & 15371881.0 \\ 676.408048 & 62122979.4 \\ 676.419374 & 45851471.6 \\ 676.445526 & 1339304528. \\ 0 \\ 676.445526 & 1339304528. \\ 0 \\ 676.468426 & 50599789.7 \\ 676.479270 & 30373811.2 \\ 676.486515 & 37018959.8 \\ 676.496340 & 23991641.2 \\ 676.505292 & 28265522.1 \\ 676.505292 & 28265522.1 \\ 676.514315 & 27569320.6 \\ 676.532633 & 111341706.7 \\ 676.543660 & 66244585.8 \\ 676.570704 & 2111879384. \\ 0 \\ 676.591682 & 77138646.0 \\ 676.611245 & 56017752.0 \\ 676.611245 & 56017752.0 \\ 676.619805 & 35327541.9 \\ 676.629566 & 38745838.0 \\ 676.67391 & 134932471.9 \\ 676.678822 & 78977449.1 \\ 676.678822 & 78977449.1 \\ 676.695805 & 2350566485. \\ 0 \\ \hline \end{array}$	676 270427	10023494.2						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	070.370127	142/0400.0						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	070.384332	1537 1881.0						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.408048	62122979.4						
676.445526 1339304528. 0 676.468426 50599789.7 676.479270 30373811.2 676.486515 37018959.8 676.496340 23991641.2 676.505292 28265522.1 676.505292 28265522.1 676.514315 27569320.6 676.532633 111341706.7 676.543660 $66244585.8676.570704$ 2111879384. 0 676.591682 77138646.0 676.611245 56017752.0 676.611245 56017752.0 676.611245 56017752.0 676.629566 3874538.0 676.629566 3874538.0 676.629566 3874538.0 676.657391 134932471.9 676.657391 134932471.9 676.657392 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676.419374	45851471.6						
$\begin{array}{c} 0 \\ 676.468426 \\ 50599789.7 \\ 676.479270 \\ 30373811.2 \\ 676.486515 \\ 37018959.8 \\ 676.496340 \\ 23991641.2 \\ 676.505292 \\ 28265522.1 \\ 676.514315 \\ 27569320.6 \\ 676.532633 \\ 111341706.7 \\ 676.543660 \\ 66244585.8 \\ 676.570704 \\ 2111879384. \\ 0 \\ 6\\ 76.691682 \\ 77138646.0 \\ 676.611245 \\ 56017752.0 \\ 676.611245 \\ 56017752.0 \\ 676.629566 \\ 38745838.0 \\ 676.629566 \\ 38745838.0 \\ 676.629566 \\ 38745838.0 \\ 676.657391 \\ 134932471.9 \\ 676.657391 \\ 134932471.9 \\ 676.678822 \\ 78977449.1 \\ 676.695805 \\ 2350566485. \\ 0 \\ 6\\ 76.712388 \\ 98535232.1 \\ \end{array}$	676.445526	1339304528.						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$		0						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	676.468426	50599789.7						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	676.479270	30373811.2						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	676.486515	37018959.8						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	676.496340	23991641.2						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	676.505292	28265522.1						
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.514315	27569320.6						
$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	676.532633	111341706.7						
676.570704 2111879384. 0 676.591682 77138646.0 676.602485 676.602485 38581643.8 676.611245 56017752.0 676.619805 35327541.9 676.629566 38745838.0 676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 0 676.712388 98535232.1	676.543660	66244585.8						
0 676.591682 77138646.0 676.602485 38581643.8 676.611245 56017752.0 676.619805 35327541.9 676.629566 38745838.0 676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676.570704	2111879384.						
676.591682 77138646.0 676.602485 38581643.8 676.611245 56017752.0 676.619805 35327541.9 676.629566 38745838.0 676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1		0						
676.602485 38581643.8 676.611245 56017752.0 676.619805 35327541.9 676.629566 38745838.0 676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 0 676.712388 98535232.1	676.591682	77138646.0						
676.611245 56017752.0 676.619805 35327541.9 676.629566 38745838.0 676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676.602485	38581643.8						
676.619805 35327541.9 676.629566 38745838.0 676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676 611245	56017752 0						
676.629566 38745838.0 676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676 619805	35327541 9						
676.638135 37636107.8 676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676 620566	38745838 0						
676.657391 134932471.9 676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676 629125	37636107 0						
676.678822 78977449.1 676.695805 2350566485. 0 676.712388 98535232.1	676 657204	124022474 0						
676.695805 2350566485. 0 676.712388 98535232.1	010.001391	1349324/1.9						
676.712388 98535232.1	0/0.0/8822	18911449.1						
0 676.712388 98535232.1	676.695805	2350566485.						
6/6./12388 98535232.1	070 740000	U DOFESSOR (
	676.712388	98535232.1						

676.735977	57888830.8					
676.743430	38234956.9					
676.753984	39163516.0					
676.762387	36657561.8					
676.782190	135459408.5					
676.798742	59106797.0					
676.820847	1997254297.					
	0					
676 860725	46553219.5					
676 878336	28267141.3					
676 886779	27660163 1					
676 907227	102686862 1					
676 922568	47285898 1					
676 945876	1411811350					
010.040010	n					
676 060582	0					
676 085820	21025276 2					
677.002045	17155472.2					
677.003043	17100470.0					
077.010910	10409/09.4					
077.021093	1/000040.9					
077.032039	7 1530844.3					
077.040890	33013990.8					
677.070880	963963387.5					
677.094343	31652416.6					
677.111923	20645959.6					
677.137091	12670373.2					
677.157634	46554603.2					
677.171432	20250897.5					
677.195922	576079625.1					
677.219610	20068370.3					
677.236802	16159955.5					
677.256205	6415461.7					
677.264974	5188949.7					
677.282556	26628410.7					
677.296078	10506439.6					
677.320901	325071932.9					
677.362171	6998622.8					
677.381444	3350581.1					
677.389528	3739625.4					
677.407635	15733209.3					
677.423273	8847064.1					
677.446092	198508193.9					
677.468717	6911910.0					
677.487278	5293095.1					
677.506029	2699582.5					
677.523533	4005081.7					
677.537127	2163110.9					
677.545980	3643438.6					
677.571123	105726269.4					
677.611501	2599049.5					
677.623226	2910797.4					
677.635895	1997353.2					
677.696235	50105838.7					
677.722206	2848457 4					
677,736037	3087685 5					
677.820732	22422530.6					
677.852572	2792964.6	C106H132N22O57P10S	677.852671	0.146	-5	d10 - NH3
5COLO. L		10	5	5.1.10	-	
677,946112	12247984.5	10				
678.071480	5548593.8					

678.196834 678.445351 678.569593 678.693505 678.819365 679.068017 679.193229 679.279147 679.318342 679.404787 679.443163 679.568268 679.693517 679.817806 679.942452 680.068072 681.064186 681.314001 681.440422 681.563700 681.689731 682.395270 690.736136 690.835788 690.936476 691.036522 727.677437 743.583622 747.737399 767.091580 767.921573 767.931630 768.252927 768.263279 770.042671 773.26061 773.610044 773.653205 778.786238 778.794185 779.507799 791.478522	3536380.4 2181286.8 2856942.2 2741105.0 2729577.9 10559204.8 22486782.5 2241412.7 32462966.6 2142412.0 30698988.8 23207713.5 13508959.9 10603946.2 6982888.2 1945161.3 1764848.4 2140946.8 1812207.1 2356112.3 1751704.1 1796795.4 2533836.5 2695622.2 2756918.8 1769547.3 2355547.0 3098158.1 2852872.5 2938220.4 2204085.1 3340896.7 2608376.5 5783073.2 2527418.5 2336579.4 3279493.3 1995741.1 3660735.6 2204170.1 2261073.8 2753107.3 4869501.5	C ₁₂₆ H ₁₅₇ N ₄₀ O ₆₅ P ₁₁ S	791.477745	- 0.982	-5	a12 - 2H, b12 - H2O
791.478522 791.683635 809.244518 809.412924 809.583106	4869501.5 5265322.7 2646074.0 2200580.8 2998124.0	C ₁₂₆ H ₁₅₇ N ₄₀ O ₆₅ P ₁₁ S	791.477745	- 0.982	-5	a12 - 2H, b12 - H2O
819.077302	2653843.8				_	
819.275993	9287857.0	C ₁₃₀ H ₁₆₅ N ₃₈ O ₆₈ P ₁₂ S	819.275150	-	-5	атз - В(G) - ОСН2
010 170050	10400424 0		010 476470	1.029	Б	w12 + 2H
819.476652	10400434.6	$C_{126}H_{162}N_{44}O_{66}P_{12}S$	819.4/61/8	- 0 E 7 9	-5	W12 + 2H
010 670047	E160140 4	12		0.578		
819.678017	5160140.4					
860.490217	984/022.2		000 00007	0.005	F	712
800.089693	1499/227.1	$C_{136}H_{172}N_{46}O_{69}P_{12}S$	800.090007	0.365	-5	213
860.890018	10153079.3	${\overset{_{12}}{C}}^{_{12}}_{_{136}}H_{_{173}}N_{_{46}}O_{_{69}}P_{_{12}}S$	860.891572	1.805	-5	z13 + 1H
861.088815	1995140.7					

			Abs mean error Abs mean std dev	1.254 1.193		
1382.88898 3	4191613.4					
2 1355.12956 3	8243090.6					
0 1354.88626 2	9707054.5					
1354.63083	11556415.2					
5 1354.39487 1	21162897.4					
0 1354.14040 5	12422843.9					
1 1353.88927	8821596.1		8	3./14		
903.103364 987.350404 987.492629 1029.43091	5340552.8 4244072.5 2520404.9 1801827.3	$C_{96}H_{122}N_{31}O_{51}P_9S_9$	1029.42708	-	-3	d9
902.512413 903.088727	2404363.3 12502482.5	C ₁₄₃ H ₁₈₃ N ₄₃ O ₇₅ P ₁₃ S	903.088442	- 0.316	-5	b14 - B(G) + 1H, a14 - B(A) + 2H
902.364671 902.418674 902.430634	2078123.6 4541622.7 4835952 5					
902.257288 902.272893	38775853.6 9774832.1					
901.927567 901.958943 902.125126	47903549.5 2013722.9 2549807.9					
884.779648 901.760280 901.860281	2827743.2 22683477.4 3628281.9					
876.915628 881.253695 884.441921	3664065.8 1825487.9 2120013.3	$C_{86}H_{107}N_{30}O_{41}P_7S_7$	884.440000	- 2.172	-3	y8 - H2O, z8 - 2H
864.169711 864.297983 876.752174	8249064.0 3699198.2 3013012.7					
863.542342 863.741353 863.909425	19006860.3 1864584.5 2606768 0					

Table S14 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of one scan denoised (sane rank 10) [M-7H]⁷⁻ precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured	Intensity	Elemental	Theoretical	Error	Charg	Assignmen
mz	-	Composition	mz	(ppm)	e	t
255.866784	3610139.0					
383.685103	6199175.2					
383.741385	3294117.3					
383.785554	1752580.9					
383.841110	4109102.5					
383.852558	32505181.8					
383.864384	3734794.7					
383.896892	5396112.4					
383.907975	37886865.6					
383.916111	2055700.2					
383.920011	4260967.5					
383.952070	4188873.8					
383.975584	3866152.2					
384.008704	2/1/526.8		004 040405	0.050	-	-0 D(T) 411
384.019105	22050820.7	$C_{61}H_{75}N_{14}O_{34}P_6S_6$	384.019125	0.052	-5	со - В(Т) - 4Н
384.031185	2687780.2					
384.074861	11964750.5					
384.130517	4955578.4					
380.082179	3568937.3					
380.753409	49/0/01.3		206 026740	1 507	F	$x \in B(dA)$
300.020135	2222030.2	$C_{60}\Pi_{77}\Pi_{18}O_{32}P_6O_6$	300.020749	1.007	-5	OCH2
601.619497	1734570.2					
676.537841	7016826.7					
676.687643	2052/18.8					
676.696758	4411/51.5					
676.703219	3615941.3					
676.910633	1837422.4		700 077004		-	011 111
728.078860	18//2/2.6	C ₁₁₆ H ₁₄₇ N ₃₈ O ₅₉ P ₁₀ S	728.077801	-	-5	
752 700262	1016602.0	10		1.455		
752 022200	1910003.0					
753.932300	2040007.0					
754.070920	2043009.7 5470247 4					
765 508616	18503178 6					
765 620524	1028865 2					
765 656558	1920005.2					
765 672307	101004437.3		765 671473	_	-5	z12 - B(dC) -
105.012501	1919040.1		100.011410	- 1 089	-0	OCH2
765 709871	35555376 1	11		1.005		
765 767521	1907022 3					
765 782199	2098160.3					
765 799707	2178243 7					
765 821254	51036461 4					
765 853199	2909196 2					
765 867040	2371613.8					
765.877658	3872165.7					
765.886565	3071598.8					
765.898209	3082407 7					
765.932594	60995960.3					
765.961240	3547901.4					
765.973399	2369344.2					

765.987063 766.006912	3572177.4 2597221.9					
766.020135	2963440.7					
766.043676 766.101621	52661330.8 3560714.2	$C_{24}H_{33}N_8O_{13}P_2S_2$	766.101098	-	-1	w2 + 1H
766.108141	3853459.5			0.683		
766.121009	2542394.1					
766 154759	45232279 5					
766.184661	3348837.5					
766.217333	3783983.4					
766.240870	2212025.4					
766.299480	2677083.8					
766.331287	3304060.1					
766.349189	2768007.0					
766.376922	24945135.7					
766.407599	2070950.1					
766.441326	2951904.9					
766.487377	17654784.0					
766.515635	2466585.8					
766.525831	2368096.8					
766.537297	2061383.2					
766.550353	2449211.0					
766.559308	2120471.4	$C_{96}H_{117}N_{31}O_{50}P_9S_9$	766.559987	0.886	-4	c9 - 4H
766.570383	2259530.8					
766.599021	13251050.3					
766.617538	2218308.5					
766.629099	2633976.1		700 000705		-	
766.664168	2337360.2	C ₁₂₁ H ₁₄₉ N ₃₆ O ₆₅ P ₁₁ S	766.662765	- 1.830	-5	b12 - B(dC) - NH3
766.674746	2803935.7	$\dot{C}_{121}H_{155}N_{39}O_{62}P_{11}S$	766.677051	3.006	-5	z12 - B(G) + 1H
766 600267	2702162.2	11				
766 700871	2702102.2					
766 727220	22082/17 2					
766 736073	2230247.2					
766 753360	6747767.9		766 754257	1 170	-3	a7 - 2H, b7 -
100.100000	07 11 101.0	0761 1951 121 0 391 606	100.101201	1.170	Ũ	H2O
766.771698	2397581.4					
766.786353	3099421.9					
766.804256	24/39/5.0					
766.821253	6274008.7					
766.854889	3120224.6		766 070054		F	212 B(T) +
/00.8/3022	3944690.7	$C_{121}H_{154}N_{38}O_{63}P_{11}S$	/00.8/3854	-	-၁	2H
766 803702	3310180 6	11		2.305		
766 01/077	3750782.2					
766 031663	1203272 8					
766 945012	3480362 0					
766 953696	3877626.5					
766 972928	3986802.1					
766.986408	3736664.8					
767.006257	4161383.1					
767.021789	4587019.4					
767.041195	4943503.7					
767.056040	4440188.1	$C_{71}H_{91}N_{20}O_{40}P_7S_7$	767.056382	0.446	-3	w7 - B(dA) -
767 114790	1005093 6					2H
767 128/57	4990903.0 5008560 2					
767 148610	6199769 4					
767,178183	6631435.9					

767.211453 767.229466 767.241873 767.262443	14350596.5 11360473.6 11618142.8 222047526.9	CurtureNacOarPurS	767 262699	0 334	-5	b12 - B(A) - 4H
101.202443	222041320.3		101.202033	0.004	-0	2.2 2007
767 285734	16870471 9	11				
767 204080	14728073 6					
767 300831	16105060.8					
767 32/213	10130303.0					
767 3/1308	31702363 /					
767 272900	716474776 7					
707.373009	22071767.0					
707.403033	72960612 1					
767 450205	15000012.1					
707.40000	40100200.4 50010106 2					
707.402000	02019120.0 1065460000					
/07.403102	1200400020.					
	U 00004000 F					
767.507995	02891909.0					
707.540037	93318894.0					
/67.596192	1630032964.					
707 000050	0					
767.626958	63195576.9					
767.641596	42681428.6					
/6/.65//9/	103963924.9					
767.672803	63905629.8					
767.687654	79314927.2					
/6/./0/599	1690442984.					
707 700000	0					
767.768268	104091117.3					
767.787465	51123877.9					
767.849930	55160123.4					
707.879429	87010450.2					
707.090200	409/0103.0					
/0/.930045	0					
767 957614	46585594 5					
767 969230	22576520.5					
767 990770	67230563.8					
768 015884	27077/67 8					
768 041067	803717200 6					
768 072482	30581480 7		768 071724		1	c9 + 2H
100.012402	30301400.7	0961 1231 131 0501 909	100.071724	- 0.087	-4	
768 101006	51124579 1			0.007		
768 119892	24950635 1					
768 152501	575466569 2					
768 181031	25714051 4					
768 197221	12122105.0					
768 213772	34202749.0					
768 228870	14851754 8					
768 242053	16719047.9					
768 263569	375054403 4					
768 325351	21962500 2					
768 344234	10093619.5					
768.374648	225181697.6					
768.404996	8933948.6					
768.436558	12055206.8					
768.455349	5435290.6					
768.485937	127447492.6					
768.514035	5404641.1					
768.527727	3639340.7					

768.549147	7324950.5					
768.570284	3546163.0					
768.625365	3858409.2					
768.633849	2940872.2					
768.658831	4602198.4					
768.680634	2541468.5					
768.708337	40545200.4					
768,744452	2123320.3					
768 756252	2637375.0					
768 785846	5096026.8					
768 819846	21464261 7					
768 8/8213	2356250 8					
768 861058	2030230.0					
768 883/68	2233310.3					
760.003400	5449109 0					
760.907701	10952440 0					
700.930041	10000449.9					
700.900001	3124943.0					
768.977440	1743895.0					
769.001672	1/50/04.1					
769.042430	8408158.8					
769.058421	2078191.4					
769.123518	1939109.5					
769.151150	5413774.9					
769.168391	4216262.8					
769.192862	2310585.3					
769.214269	2024984.7					
769.239337	2228859.8					
769.288731	3766648.3					
769.348754	1818052.7					
769.375186	10234975.2					
769.405938	2164215.5					
769 446332	1776330 1					
769 485397	7742042.9					
769 500301	1879278.4					
769 526629	2170282.7					
760 5610020	1838636 5					
769.501900	6705018 5					
760 705747	14070550 7					
709.703747	2142160 2					
769.770630	3143109.2		700 047500	1 661	4	V0 CH3
709.810281	32895378.3	$C_{95}H_{118}N_{35}O_{48}P_9S_9$	/09.81/500	1.001	-4	X9 - CH3
769.882409	3400520.3					
769.892109	2195158.0					
769.906108	2/1146/./					
769.927434	56965789.5					
769.949600	3591183.2					
769.987954	4555290.0					
770.014085	2469194.1					
770.038721	63744751.3					
770.072269	3006868.8	C ₁₂₁ H ₁₅₄ N ₃₈ O ₆₄ P ₁₁ S	770.072837	0.738	-5	b12 - B(T) +
		11				1H
770.093603	6328890.7					
770.118141	2582463.2					
770.150107	69517503.3					
770.180385	3474300.3					
770, 192682	2350741.3					
770.206681	4324717.2					
770 238158	5340077 5					
770 261286	62787818 8					
770 283040	3909304 0					
770 335007	2306580 0					
110.000002	20000000.0					

770.348724	2811847.9					
770.392852	3976690.0					
770.405508	2712759.1					
770.451933	2257352.4					
770.483733	36138896.2					
770.524356	3155632.4					
770.540315	2559077.7					
770.560418	2234250.8					
770.594812	23699270.0					
770.633909	1784288.4					
770.650968	2221250.5					
770,084950	21080000.0					
770 726334	14004233.7					
770 766188	19390493.1					
770,798907	24187683.1					
770.893512	2966109.0					
770.921240	4562337.3					
770.942588	46568039.5					
770.962921	2799686.3					
771.035352	5590677.4					
771.049159	3666918.0					
771.085193	59925657.0					
771.106770	2398310.6					
771.142471	2327309.7					
771 10/566	4700517.9 270/168.0					
771 227948	58908944 5					
771 250695	2798139 7					
771.269583	2161028.1	C121H150N41O62P11S	771.270456	1.132	-5	z12 - B(dC) -
		11				2H, y12 -
						y12 - B(T) -
	0555005.0					NH3
771.320716	2557635.0					
771.371094	54764215.9					
771 51/000	1022034.7					
771 591661	12613808 5					
771 622774	1831336 4					
771.656592	26473407.7					
771.701560	20897044.0					
771.746666	3179007.9					
771.756016	3483587.1					
771.795643	12751182.4					
771.814571	24295743.9					
771.891348	2083498.0					
771.923591	25783260.5					
771.944881	6454570.9					
772 034775	2930939.4					
772 084804	7680307 7		772 085896	1 4 1 4	-3	b7 - 2H
772.145567	18372652.0	0761 1951 121 0401 606	112.000000	1.414	-0	
772.229021	2115000.0					
772.257316	10922988.3					
772.368337	11085910.6					
772.416546	1955829.0					
772.479130	5815891.0					
772.592757	2907802.0					
770 70 5000	0000004 4					

773.000791	1952490.0					
773.031008	9392357.1					
773.045547	5551434.7				_	
773.081488	127140707.3	$C_{172}H_{217}N_{56}O_{88}P_{15}S$	773.079889	2.068	-7	M - 7H
772 10/221	5061701 0	15				
772 125105	0901721.0 5552240.1					
772 144040	0000249.1 1605261 0					
772 450702	4000001.0					
772 174700	4730291.1					
773 100500	02221022					
773 224209	9000102.0 245561126 4					
773 255030	10/01533 2					
773 267655	10401000.2					
773 200371	60690137					
773 316615	19448748 2					
773 336597	10023743 5					
773 367293	296464981 4					
773.399528	9724953.4					
773.419626	6574535.0					
773.459749	15575045.0					
773.475287	8333916.7					
773.510381	255206763.6					
773.563158	7404690.9					
773.574686	4550694.5	C ₉₆ H ₁₂₁ N ₃₅ O ₄₈ P ₉ S ₉	773.573428	-	-4	x9
				1.626		
773.587258	4687840.0					
773.601978	12713446.9					
773.620623	7363045.5					
773.653336	173606790.6					
773.683711	6840504.6					
773.705953	4676020.8					
773.720107	3487264.2					
773.744849	10407017.5					
//3./96/14	99049298.4					
//3.849/33	3530281.7					
773.887351	7373780.9					
773.905343	3502723.6					
773.940377	57730249.1 2456200.0					
772 00/552	2430300.0					
774 022026	1014007.1					
774.033020	4040309.0					
774 225045	1021/788 3					
774 367563	5544808 1					
811 076521	3087090 5					
817 541991	1829962.6					
838 161227	3411936.0					
838 289210	8026811 8					
838.663364	2149612.8					
863.547208	2107692.7					
864.293701	3903138.8	C136H174N46O70P12S	864.292120	-	-5	y13 + 2H
		12		1.829	-	
902.750562	2065263.0	-				
908.535000	2468512.2					
908.699141	5235373.3					
908.871934	5017438.0					
909.041090	2628007.0					
958.041309	2042295.6					
958,186695	2220046.3					

967.333684	1864564.3					
967.470591	4661105.1					
967.613112	5874718.9					
967.758174	5589847.4					
984.192873	5086973.0					
984.336008	7175087.2					
984.479466	4749622.4					
986.481750	3661598.7					
986.622582	11994536.6					
986.766019	12423686.2					
986.896634	5962200.5					
986.915472	4606523.7					
986.962939	3561800.9					
986.991586	2741168.2					
1024.34627	378492.0	$C_{126}H_{161}N_{44}O_{66}P_{12}S$	1024.34508	1.156	-4	w12
0		12	6			
1082.31115	2150783.8	C ₁₇₂ H ₂₁₅ N ₅₆ O ₈₈ P ₁₅ S	1082.31162	0.439	-5	M - 7H
1		15	6			
1082.51296	5040763.8	C ₁₇₂ H ₂₁₆ N ₅₆ O ₈₈ P ₁₅ S	1082.51319	0.210	-5	M - 5H - 4H
4		15	1			
1082.91343	2786627.3					
8						
			Abs mean	1.287		
			error	0.074		
			Abs mean	0.371		
			std dev			

Table S15 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of one scan and no denoising of [M-8H]⁸⁻ precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured	Intensity	Elemental	Theoretical	Error	Charg	Assignmen
mz		Composition	mz	(ppm	е	t
)		
225.564620	4432978.2					
338.157835	11445873.4					
338.211348	3663335.9					
338.220331	25879588.2					
338.229994	3355645.6					
338.274159	3407926.9					
338.283009	30083773.9					
338.292559	4503527.9					
220 200622	2570002 7					
330.399033	16206257 6					
338 /62176	3122/36 1					
338 /70632	228//711 0					
338 470713	2078684 4					
338 533138	18663184 5					
338 595374	7109467 6					
338 658348	4542706 1					
338 720810	3274095 5					
383.685875	3005234.7					
383.741421	3047159.4					
383,796819	4790834.8					
383.852803	5536303.5					
383.908368	5491036.3					
384.019223	3684546.1	C ₆₁ H ₇₅ N ₁₄ O ₃₄ P ₆ S ₆	384.019125	-	-5	c6 - B(T) - 4H
				0.255		
386.611177	4820919.8					
386.682538	5937741.5					
386.753958	6352443.1					
386.825573	8437067.5					
386.897146	5341620.1					
386.968404	3150199.8					
431.773017	4/306/3.5					
431.898246	5619314.3					
432.023441	4464920.4					
451.215020	3808400.0					
401.290402	3200024.0					
401.301033	4227430.0					
493.070900 541.054566	5112/10 2					
541 254315	8222990 8					
541 454155	3680355 6					
599 619888	4344628.6					
601 061588	8656425.0					
601.174444	5866803.3					
601.284159	16500222.7					
601.395476	34268726.7					
601.507165	8021247.4					
601.618941	6016479.6					
601.729300	9369557.5					
601.839552	7788598.0					
601.951839	5511524.5					
609.308719	3498098.6	$C_{76}H_{98}N_{25}O_{40}P_7S_7$	609.308004	-	-4	w7

627.759577 627.850219 627.940275 628.032667 628.122957 628.213923 657.594697	4309770.9 9953375.3 4212455.1 4878836.6 7767706.6 8919933.7 4015166.8			-		
658.097654	3147957.1	$C_{46}H_{57}N_{12}O_{22}P_3S_3$	658.096992	- 1.006	-2	a4 - 2H, b4 - H2O
659.438524 659.565209 659.689487 659.815102 659.938912 660.065225 674.323209 674.448375 674.573862 674.698952 674.698952 674.824210 674.948450 675.073082 675.198264 675.323832 675.447059 675.573081 676.203057 676.235137 676.252071 676.260528	3071434.2 4559483.4 10067982.4 10005065.3 5867082.1 3170077.0 8000287.7 15905799.5 22584435.9 29111250.8 27052144.4 22368125.9 13090907.2 12758975.4 6824854.3 6258253.2 3518445.4 3619655.6 3746144.8 4930792.5 4361064.3			1.000		
676.283233 676.295047	15564328.4 13978909.4					
676.320091	449150480.4	C ₁₇₂ H ₂₁₇ N ₅₆ O ₈₈ P ₁₅ S	676.318994	1.622	-8	M - 8H
676.344306 676.361047 676.377876 676.384426 676.408122 676.419286 676.445508	17375037.8 13575618.6 11799169.8 12660860.3 51817222.3 38577327.3 1125225782. 0	15				
676.468474 676.479285 676.486520 676.496293 676.505410 676.514228 676.532749 676.543426 676.543426	42438058.5 25792906.1 31552394.5 20415786.4 23584962.5 23659985.2 96512871.7 57886550.8 1854525468.					
676.591763 676.602591 676.611250 676.619765 676.629611 676.638140 676.657565	0 67891764.3 34444926.7 50285717.1 31839898.8 34173202.1 33858821.0 123383411.1					

676.678658	72503957.9
676.695817	2194204109.
676.712473 676.735930 676.743475 676.753936 676.762426 676.782225 676.798739 676.820855	92581427.3 53893085.2 35533788.2 35644811.2 33900224.8 123855911.6 55555879.8 1881691596. 0
676.860665	43596738.0
676.878265	26271431.8
676.886799	25808664.7
676.907262	96441757.6
676.922539	44874404.5
676.945864	1367774834.
676.969571 676.985673 677.003062 677.010939 677.022231 677.032647 677.070872 677.094309 677.111897 677.136865 677.144009 677.157598 677.171331 677.195905 677.219668 677.236566 677.236566 677.236566 677.236566 677.282545 677.362266 677.370223 677.362266 677.370223 677.381813 677.389304 677.389304 677.407740 677.423289 677.446116 677.468612 677.468612 677.535502 677.545883 677.545883 677.571105 677.611658 677.625464	U 41636412.8 30560242.8 16845822.4 18294069.7 17719845.6 72450755.7 33768785.6 979973286.7 32020874.3 21296088.3 12897723.1 9559570.0 48633516.6 21147556.3 609568604.6 21197933.7 17549782.8 6681177.4 29079974.9 11749361.1 368877443.3 6548642.7 8076596.7 4052381.7 4043024.1 4311724.4 17570670.6 9723876.0 224005489.8 7681294.4 5827285.7 3246821.6 4992724.3 3766772.5 4228614.9 123068616.8 3213044.1 3709773.3
677.653864	3176321.5
677.696212	63732994.3

677.723426 677.735208 677.820878 677.946207 678.071266 678.196739 678.445709 678.693885 678.819348 678.944997 679.068047 679.114395	3545545.5 3868673.0 30403183.3 16751425.8 7971883.2 5036525.6 4016997.9 5463928.6 5241741.7 5408154.5 3872184.4 24832625.0 4429997.1	C46H59N16O21P3S3	679.113507	-	-2	у4
679.153132	3502811.8			1.500		
679.193252	52406402.9					
679.279432	4768727.1					
679.318261	75526728.3					
670 442220	0100009.4 70771102 0					
679 530104	4421684 3					
679.568303	66169948.9					
679.655051	3253925.7					
679.693372	43781992.0					
679.818021	32391928.0					
680 068052	20013230.0					
680.193433	4785558.0					
680.318176	3892605.5					
681.063513	11632771.4					
681.188856	18496986.8					
681.314435	18693358.4					
681 564119	21443351.0					
681.689650	10176818.7					
681.813423	5387611.2					
681.939208	3786467.5					
682.062928	4821061.4					
682.189181	3129427.3					
689 237404	2960416 9					
690.536404	3796913.0					
690.637266	7171002.3					
690.737707	10067253.2					
690.835657	7314165.4					
690.937544	21346003.6					
691 134381	4841259.0					
691.236439	11396104.8					
691.436154	4001922.2					
727.674371	2958368.1					
743.583147	3318186.7					
/4/.738727	32/9538.1					
101.930201 752 <u>1</u> 80511	2909202.0 3337064 5					
752.703341	3912309.1					
753.933122	4763156.9					
754.074165	4391564.8					
754.218145	6446065.6					
754.360903	4905642.0					

754.503212	3918422.1					
754.642698	3241700.4					
755.949066	3085865.7					
765.713901	3015591.0					
765.821212	4636514.9					
765.931197	5354531.1					
766 756875	3774977 1					
767 091342	4751358 5					
767 327565	4075465.6					
767 372695	6662063.8					
767 438712	5727800.7					
767 485757	/0111102.8					
767 507/85	3/30208 1					
767 548203	61/0/3/ 1					
767 506469	30622612 5					
707.090400	7650207 2					
707.000429	1050291.5					
707.700002	40000420.7					
767.772509	4009873.0		767 040760		4	c0 ± 1⊔
/0/.820340	15820792.0	$C_{96}H_{122}N_{31}O_{50}P_9S_9$	/0/.819/08	-	-4	C9 + 111
707 0000 40	7574005 0			0.753		
767.883219	/5/1085.8					
767.930113	52225490.5					
767.994344	4621573.5					
768.041399	28432899.3					
768.152488	11003381.3					
768.263684	24557870.4					
768.376086	7405030.5					
768.487577	4633303.9					
768.597278	3803506.4	$C_{51}H_{65}N_{15}O_{25}P_4S_4$	768.598191	1.188	-2	z5 - B(dC)
770.037994	4613908.7					
771.086252	6162871.1					
771.229439	3639209.2					
771.371454	4141501.4					
771.480254	3051724.1					
771.512642	3112167.3					
771.810447	3834877.5					
772.079459	3128801.6					
772.146820	3648785.7					
772.258881	3185871.0					
772.369548	4125983.9					
772.937599	3873390.9					
773.035226	3706450.5					
773.081950	13595266.5					
773.177474	5216293.9					
773.224417	40518666.5					
773.321132	7585378.5	C96H120N35O48P9S9	773.321472	0.440	-4	w9 - H2O
773.367808	60433856.8					
773.463261	10037742.9					
773.511871	59768503.3					
773.533829	4299998.9					
773.606560	10726315.5					
773.654091	83322937.5					
773.699648	3166241.0					
773,749997	7011783.9					
773,796710	13536684 3					
773.891166	5934787 2					
773 939372	39965491 1					
774 083324	19880479 9					
774 227015	11857823.3					
774 366218	5327461 7					

774.511674	5821579.8					
774.796242	3259120.1					
776.507992	4873977.6					
776.651848	7272871.6					
776,794065	10244021.7					
776,939979	3965695.4					
777 220008	3267660.9					
778 645883	3848342.0					
778 788603	7766015 7					
778 0318/1	6200034.2					
770.931041	6717275 0					
770 00000	2276965 4					
770.250024	32/0003.4					
779.308924	3407473.4					
779.503890	0413121.0					
779.649536	3877925.5					
791.480491	4957579.2					
791.680195	5084228.8					
791.880441	7388811.7	C ₁₂₆ H ₁₅₉ N ₄₀ O ₆₅ P ₁₁ S	791.880875	0.548	-5	a12
		11				
792.080059	4727376.4					
809.245586	3188481.8					
809.581634	3653078.4					
817.020900	4317702.0					
818.111884	3223753.8					
819.075977	3781586.2					
819.476516	8527175.5	C ₁₂₆ H ₁₆₂ N ₄₄ O ₆₆ P ₁₂ S	819.476178	-	-5	w12 + 2H
		12		0.412		
819.677058	5419794.0	12				
824.089062	3233847.2					
838.411777	3431233.0					
838 537347	4435107 5					
846 663462	3741691.8	$C_{420}H_{40}N_{44}O_{70}P_{40}S$	846 664127	0 785	-5	x13 - B(A) -
010.000102	07 1100 1.0		010.001121	0.100	Ũ	OCH2
846 791853	3629964 7	13				
8/6 016257	5/67/75 8					
847 040030	3450616 5					
847 164643	33/5080 1					
847 280700	11/2101 0					
047.209799	2075426 1		017 112151	0.042	2	v8 - B(dC) - 4H
047.413413	0104750.1	C ₈₁ Π ₉₈ Ν ₂₇ O ₄₁ F ₇ S ₇	047.413451	0.042	-3	yo - D(do) - 411
000.409013	9124759.4		960 600007	0 170	E	713
000.009009	14405027.4	$C_{136}\Pi_{172}\Pi_{46}O_{69}\Pi_{12}O_{69}$	000.090007	0.172	-0	215
004 005070	20200405	12				
861.295973	3020640.5					
861.548676	3338284.0					
861.798825	3434080.8					
861.924666	3844193.1					
862.049519	4802487.8					
863.296088	12759855.3					
863.363628	3661256.2					
863.420977	27455807.5					
863.489387	6715713.5					
863.546631	70618663.7					
863.613198	7146466.5					
863.670950	56701990.6					
863.698056	3253742.5					
863.737574	10682828.9					
863.795006	31811137.4					
863.865869	5350471.7					
863.923245	29593047.1					
863.988833	4372746.3					

864.047536	30018786.0					
864.110425	3784236.5					
864.173549	43117996.7					
864.235732	3123675.6					
864.298399	27580100.5					
864.421056	6699241.2					
864.547593	5507905.3					
866.295316	4193850.2					
866.417793	3178036.7					
866.545327	5155109.7					
866.669188	3226038.5					
866,795660	3161346.2					
867.044390	3155638.7					
868,287636	3286253.3					
868 412479	3498312.4					
868.541329	5402233.4					
868,666835	4027127.6					
868 792992	4058035.3					
868 918110	4225133.6					
876 918359	3996472.5					
877 086806	5093324 0					
877 253681	3496399.8					
881 424382	2070311 2					
881 76358/	2979311.2		881 76/150	0.642	3	b8 - H2O a8 -
001.703304	3230390.1	C861 1107 N26 C44F 7 S7	001.704150	0.042	-3	2H
884.778014	3323110.3					
887.099082	3286911.0					
887.601312	3051364.7	C ₅₆ H ₇₄ N ₁₈ O ₂₉ P ₅ S ₅	887.600761	-	-2	w5 + 1H
				0.621		
899.933646	3546896.0					
900.102401	3203339.7					
900.266378	3775906.6					
901.760290	17253985.4					
901.860425	3075151.3					
901.927539	39659553.8					
902.032055	3632398.6					
902.094362	54426803.6					
902.125287	3090601.0					
902,199346	5273139.5					
902.261185	51670610.6					
902,288316	3391364.5					
902 363916	8869288 8					
902.428900	50566165.0					
902 529753	6169131.9					
902 598009	46777023.9					
902 699884	4626140 1					
902 764983	25456028.9					
902 865066	3999736 7					
902 930351	26276175.8					
903 032390	4451918 8					
903 096045	37038230 8					
903 198117	3173038 1					
903 264690	13219065 6					
003 1204030	13155618 0					
903.400004 903.507312	11467/02 /					
006 257/10	3866025 0					
006 020125	3000920.9					
008 7525100	5005223.2 5207760 1					
900.733519	3201103.1		000 080380	0 300	_1	a11 - 4H
909.000990	5250425.1	U116I I142IN38U59F 10U	303.003203	0.522	-4	
000 200776	3358145 0	10				
303.200110	0000140.0					

909.255000 922.759516 967.902186 968.044343 984.908281 985.054354 985.198640 985.337275 986.766406 986.910824 987.054617 987.120747 987.120747 987.195943 987.262958 987.340632 987.402788 987.402788 987.402788 987.4632 987.626065 987.767688 987.912080 988.055396 988.198773 990.049628 990.338864 990.479634	5205431.8 2983369.2 3698548.3 3265220.3 3410037.1 2951388.9 3158064.3 3211890.8 4841165.6 15449642.8 8954735.1 3797546.3 19475001.5 3194815.5 19123306.7 3268537.8 31847439.1 22278877.5 10665400.8 11273522.3 9337844.1 3236598.0 4432301.6 3349697.0 3010650.7 3412538.6	C ₈₆ H ₁₁₁ N ₃₀ O ₄₄ P ₈ S ₈	922.760626	1.203	-3	w8 + 1H
993.332789	3130027.9	$C_{121}H_{155}N_{41}O_{65}P_{12}S$	993.332314	- 0.478	-4	w12 - B(dC) + 2H
1075.11078 3	3795588.7	$C_{71}H_{90}N_{16}O_{38}P_6S_6$	1075.11031 9	- 0 432	-2	b7 - B(G) - H2O
1075.61322 7	2951800.4	$C_{71}H_{91}N_{16}O_{38}P_6S_6$	1075.61423 2	0.934	-2	a7 - B(G)
1082.71432 2	7106031.2	$C_{172}H_{217}N_{56}O_{88}P_{15}S$	_ 1082.71475 6	0.401	-5	M - 5H
_ 1082.91455 4	5968386.2	15				
1083.11376 3	9363014.9					
1083.31461 6	10429991.8					
1083.51760 1	13720642.1					
1083.71723 1	4125360.4					
1084.31631	3253062.3					
5 1084.51598	5229828.9					
3 1087.71178	4392981.0					
4 1087.91346	3327117.0					
6 1090.50320	4306057.1					
5 1091.10801	4152528.7					
∠ 1136.14118	3152910.8	$C_{36}H_{46}N_{13}O_{18}P_3S_3$	1136.13860	-	-1	w3
4 1151.39163 8	5036415.6		U	2.274		

1151.56271 5	5714845.0					
1151.72844	11301959.5					
o 1151.89362 7	6484243.1					
, 1152.06336	11121553.6					
2 1152.22775	7846277.0					
0 1152.39079	5152490.3					
5 1152.56140	5474172.8					
8 1152.72933	7238225.8					
4 1152.89567	3983254.1					
5 1353.89080	17725725.2					
4 1354.14186	24843253.8					
o 1354.39266	31627753.6					
3 1354.64265	28219927.4					
0 1354.89054	19147704.5					
3 1355.14254	18588466.7					
9 1355.39081	5421681.9					
1355.64078	4497913.3					
9 1382.06650	3677089.1					
1382.47231	5281479.5	$C_{131}H_{170}N_{38}O_{70}P_{12}S$	1382.47308	0.562	-3	b13 - B(G) + 2H
0 1382.67964	5580804.9	12	7			
0 1382.87494	6145954.1					
o 1383.07393 5	5358626.2					
1383.27494	3489990.7					
0 1383.47364 4	3775984.9					
4 1861.76720 7	4008873.3					
, 1861.90720 6	7424810.1					
U			Abs mean	0.836		
			Abs mean std dev	0.561		

Table S16 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of one scan and no denoising of [M-7H]⁷⁻ precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured	Intensity	Elemental	Theoretical	Error	Charg	Assignmen
mz		Composition	mz	(ppm	е	t
257 7/3018	305/017.6)		
257 838549	4470294 5					
257 885957	4440145 0					
338 220557	4536924.0					
338 283188	8243577 1					
338 345524	4541607 9					
338 408288	3758850 7					
338 470372	3859704 5					
338.533449	3730898.6					
383 741607	4629790 9					
383,796928	3932545.8					
383.853130	3907723.9					
383,908333	8106623.7					
386.539011	6105768.6					
386.610846	9267559.3					
386.671008	4181881.4					
386.682377	25209057.9					
386.694857	4064044.6					
386.742643	4852775.4					
386.754026	32154720.5					
386.766252	4894855.4					
386.825202	21541311.3					
386.837830	3623072.6					
386.896866	18987130.9					
386.909253	3313955.6					
386.967973	6591003.0					
387.111120	9901828.0					
387.182522	5892286.1					
387.254094	3675868.3					
431.773069	3096885.6					
431.835562	4168550.4	$C_{70}H_{86}N_{18}O_{38}P_6S_6$	431.834731	- 1.924	-5	a7 - B(dC) - CH3
431.897815	4548378.6			1.021		
451.299125	3199415.0					
451.381818	3909722.6					
493.671343	3096599.1					
541.054834	3822943.9					
541.154239	3226515.8					
541.558064	3112684.4					
601.062245	4380772.9					
601.173569	11183086.7					
601.285089	15183211.9					
601.394608	19315669.2					
601.505789	25583675.3					
601.616886	14428755.7					
601.728315	12399125.9					
601.838914	4895505.1					
601.951441	8095568.1				_	
602.061745	5360282.7	$C_{96}H_{117}N_{35}O_{47}P_8S_8$	602.062878	1.882	-5	y9 - 4H
627.669575	3232722.6					
021.159010	0092230.0					
021.049101	5104171.8					

627.940575 628.033012 628.122889 628.214427	8710254.6 5637448.0 3371172.4 6858322.0					
658.096656	3459640.5	$C_{46}H_{57}N_{12}O_{22}P_3S_3$	658.096992	0.511	-2	a4 - 2H, b4 - H2O
674.449289	4831828.8					1120
674.574816	4556358.6					
674.699396	6832336.4					
674.824621	3796775.0					
674.947002	3879218.2					
675.198501	4038278.8					
676.285094	3269783.1					
676.320460	15551372.8					
676.408716	8884701.3					
676.445731	73087061.5					
676.533198	10231596.6					
676.570584	68691221.6					
676.659715	6648565.7					
676.695159	34438424.9					
676.784033	7201544.9					
676.821493	51598120.0					
676.910040	5379938.8					
676.948449	11878370.1					
677.036246	3857524.8					
677.070495	41917446.8					
677.159310	3697258.5					
677.196747	27866366.9					
677.320401	10866290.4					
677.446515	5288286.2					
677.572423	6276702.2					
677.697586	3186574.0					
677.821797	3185150.8					
679.067430	3066444.9					
679.193390	4274700.7					
679.319817	3197339.3					
679.445885	3005778.1					
679.568462	3365939.6					
679.817879	4533850.0					
601 100117	5101114.0					
601.109117	5730013.5					
681 / 38503	5244729.0					
681 564584	7208783 6					
681 689206	6500138.4					
681.815089	3870640.1					
690.535601	16609825.2					
690.635542	10384274.5					
690.736866	25747169.9					
690.836519	26804443.9					
690.934715	19968697.2					
691.035930	19076640.4					
691.137942	7118024.1					
691.236319	10507995.0					
691.335550	8622694.8					
691.438021	5224004.4					
693.136206	3280168.8					
752.077346	3085700.5					
/52.588969	3210466.5					
/52./01511	40/6241.8					
102.012091	4293192.4					

752.923264	3461498.7					
753.146383	3211561.2					
753.788654	7345333.4					
753.932869	17422002.3					
754.075353	23308653.3					
754.218061	12780099.7					
754.361153	10235168.8					
754.503512	5141778.4					
754.645626	4093328.0					
/54./88/5/	4739214.9					
755.647109	3517469.1					
765.709599	5724461.3					
765 022007	3030032.Z					
766 042619	6110333.4 5502090 0					
766 153/61	1756801 1					
766 /88605	328070/ 1					
766 756694	3510616 3					
767 374521	25601728 5					
767 485537	36202389 7					
767 595153	57795763.0					
767.661739	5616130.5					
767.707687	84590585.9					
767.774450	4464286.9					
767.819951	28933444.3	C ₉₆ H ₁₂₂ N ₃₁ O ₅₀ P ₉ S ₉	767.819768	-	-4	c9 + 1H
		00 122 01 00 0 0		0.238		
767.885116	4744660.9					
767.927401	17248571.7					
767.996047	4314929.1					
768.039620	21597257.3					
768.106318	3080580.4	$C_{51}H_{66}N_{16}O_{24}P_4S_4$	768.106183	-	-2	z5 - B(T)
				0.176		
768.152220	34310910.8					
768.264170	9055329.6					
768.376738	10869930.4					
768.800416	3758458.3					
768.820115	3221256.2					
709.927350	4305951.7					
770 140222	0903022.2 9157967 2					
770.149222	10106314 5					
770.201029	0600075 6					
770 /83732	4074667 0					
770 594598	5777336.3					
770 703384	3687287 5					
770 798818	3878533.8					
770,942369	17549308.0					
771.084975	25017550.0					
771.228421	29087617.4					
771.370711	31061934.6					
771.486215	3422544.6					
771.513797	23583326.7					
771.591547	7413004.7					
771.656488	21175190.5					
771.702004	19395433.4					
771.756455	3202968.4					
771.796379	11102816.8					
771.814831	26510497.7					
771 002001						
111.923001	30397259.0					

_

771.983577	3178561.7					
772.034625	33634421.4					
772.145692	28637608.8					
772.226790	3272657.3					
772.235932	3433782.1					
772.257570	22152962.6					
772 368136	16950607 1					
772 415600	3316702.0					
772 470845	11032008 8					
772 502078	7029719.9					
772.393070	F920710.0					
772 762002	4006062.0					
772.703002	4990902.0					
772.797152						
772.819161	3938595.1					
//2.8380/4	3199515.0					
//2.85/160	3034624.6				_	
772.873790	3120125.9	C ₁₂₁ H ₁₅₄ N ₃₉ O ₆₄ P ₁₁ S	772.873452	-	-5	y12 - B(A)
		11		0.437		
772.891317	3577380.1					
772.906459	3613432.9					
772.930157	3395018.0					
772.944777	5176003.9					
772.952976	4758900.2					
772.967082	5496038.6					
773.002006	6776294.0					
773 031651	27394671.8					
773 044918	20443934 3					
773 060239	25253770.6					
773 08130/	511211552 7		773 070880	1 830	_7	M - 7H
110.001004	J++2++JJ2.1	C1721 12171 156 C881 15C	115.019009	1.000	-1	
773 13/770	21/25011 2	15				
772 1/5120	10256027 4					
772 150052	19230027.4					
772 475460	21304002.7					
773.175109	10352008.0					
773.190466	48945930.3					
773.224486	1291497066.					
	0					
//3.255051	53273660.0					
773.268617	26489516.8					
773.278823	39491350.4					
773.290586	33643003.1					
773.317375	111483969.7					
773.336008	64310615.4					
773.367399	1956203527.					
	0					
773.399689	64954835.9					
773.420525	44841276.0					
773.435755	31806716.4					
773.460283	141616830.2					
773.473812	76827231.6					
773 510628	2159600873					
	0					
773 533755	82603847.0					
773 563975	618755/20					
773 57/002	38707802 9		773 572100	_	_1	x9
113.31400Z	30101003.0	0961 1121 N35048F939	113.313420	- 0 740	-4	10
773 597630	39109055 1			0.742		
113.301029	30400933.4					
113.003098	13/90//90.4					
773.620103	13584558.6					
113.653476	18/0845730.					

	0					
770 604004	0					
113.084224	69499731.3					
//3./0///5	45233435.6					
773.720204	34081108.1					
773.745161	121203503.0					
773 771013	44580805 9					
770 706004	40000000.0					
113.190324	1309702825.					
	0					
773.828507	41609164.8					
773.849391	35744197.2					
773 888484	85774045 7					
772 005512	20177700 5					
773.905512	304/1/00.5					
773.939281	961637709.0					
773.968162	36531780.1					
773.982234	16002425.0					
773.993364	26497284.5					
774 004315	16558688 1					
774.004010	F4604594 0					
774.031013	04094004.Z					
774.050888	23926512.7					
774.081924	632774415.0					
774.113776	20627469.2					
774.135308	15555129.6					
774 150192	7548584 6					
774.130132	22120467 4					
774.174139	33139407.4					
774.190593	13193571.1					
774.225084	368702019.5					
774.278173	10262201.3					
774.288616	6237152.6					
77/ 303007	5130/27 /					
774.000001	20254722.4					
774.317581	20354733.0					
774.336332	9044983.3					
774.367625	233899670.6					
774.398841	7403915.3					
774,422325	4911178.5					
774 459967	10854660.0					
774 540025	10004000.0					
774.510955	120003093.1					
774.531660	5414047.7					
774.563952	3028036.0					
774.598839	5184823.9					
774.653703	72817224.8					
774 747840	6654400 4					
774 706970	38008384 2					
774.790072	10100004.0					
//4.9402//	19460013.4					
775.082998	14836975.3					
775.105197	3312431.3					
775.224193	6146969.4					
775 251424	56755694					
775 346205	3/62031 2					
775.040290	5402931.2					
775.365444	5923559.3					
775.415799	3692257.4					
775.509368	4980711.1					
775.651729	7430275.8					
775 683100	4393480 9					
775 70/0/0	0/67530.2					
775 050504	3407333.Z					
115.852504	3001/33.0					
115.937916	7970665.4					
776.082241	5718293.9					
776.170329	3172952.3					
776 221483	42733631 5					
776 274389	3167824 0					
	5.5.027.0					
776.313517	6640415.1					
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776.330479	3953219.8					
776.364678	95115493.5					
776.393825	4363988.6					
776.420185	2995037.9					
776.456378	10263386.9					
776.482621	4214725.2					
776.507488	128444299.7					
776.528721	6747355.6					
776.561027	4120818.8					
776.570451	3049638.1					
776.599104	10050151.7					
776.617371	5923226.6					
776.650423	142473468.4					
776.681658	5843923.9					
776.705166	3573768.8					
776.742400	10604913.4					
776.758314	4571394.7					
776,793336	121760019.6					
776 846784	3511206 7					
776 885502	7354180 2					
776 905564	3455114.8					
776 935997	90752218.0					
777 028900	4735807 7					
777 079187	58290809 8					
777 172440	3119100 6					
777 221843	36278248.0					
777 364284	19305211.8					
777 507942	11071205.6					
777 649732	4196602 6					
778 079414	3957644 9					
778 502388	26005226.8					
778 590434	4024816.9					
778 645592	44797787 1					
778 742568	8270869.9					
778 788833	74074741 7					
778 880027	5466502.9					
778 931657	66026108 9					
779 022518	4498825 3					
779 074242	52826020.0					
770 165031	4082560 0					
770 217231	37807437 8					
779 360142	26094613.4					
779 502775	13932460 8					
779 645547	8753264.3					
779 789467	5190608.6					
785 240832	4020643.9					
819 474598	3167699 5	Cualture Nu OcePueS	819 476178	1 928	-5	w12 + 2H
	010100010	120. 1102. 44 0 00. 120	0101110110		Ū	
819.675744	3306360.9	12				
838 286818	3596167 7					
838 540387	3326377 7					
847 164697	5544884 8					
847 290049	3106252 4					
848 041220	3516253 7					
858 078859	3348134 4					
858 245931	4301522 7					
861 424225	3174948 0					
861 545404	4917167.5					
861.675885	3351916.1					

861.799066 861.926247 862.047084 862.173959 862.298911	4338150.2 7133959.6 4679740.8 6549358.4 3900412.8					
863.294908	6857935.7					
863.421897	18436727.9					
863.485038	3725184.6	$C_{136}H_{170}N_{46}O_{70}P_{12}S$	863.485860	0.952	-5	y13 - 2H
863.550536	15423093.6	12				
863.606030	3038803.3					
863.673384	35359392.5					
863.738775	4649346.2					
863.797382	23715647.9					
863.862342	5749217.7					
863.923008	20216200.7					
863.989063	5384521.0					
864.045614	33730529.3					
864.110900	3755997.9					
864.170644	31426406.1					
864.297230	10268272.1					
864.423670	4386946.8					
864.548533	6652309.5					
864.671123	4265382.1					
866.419410	5060901.6					
866.545614	4554690.8					
866.794296	4026703.1					
866.921676	4045925.6					
868.286379	3092324.5					
879.921558	3122296.7					
880.256587	3299492.1					
881.429472	3629105.4					
882.098480	5568694.9					
882.433468	3944008.3					
887.099613	5274598.1		007 000704	4 557	0	wE + 111
887.599379	3594033.9	$C_{56}H_{74}N_{18}O_{29}P_5S_5$	887.600761	1.557	-2	W3 + 1H
902.094031	3173429.0 4101772 7					
902.201155	4101//3./					
902.201157	37/7802 0					
902.309090 002.428117	3/385801 5					
902.420117	42556164					
902 598862	23433822.2					
902 694875	5172260 1					
902.764576	35348980.2					
902.863224	3718916.9					
902.933822	7416807.1					
903.095854	28958001.7					
903.261844	21830635.0					
903.430702	4806344.7					
905.925429	3073164.0					
906.260135	5627168.8					
908.753685	5611756.3					
909.594171	3155045.0	$C_{116}H_{144}N_{38}O_{59}P_{10}S$	909.593201	-	-4	a11 - 2H, b11 - H2O
000 845600	1318310 5	10		000.1		
922.425050	5918341.6	C86H110N30O44P8S0	922.424684	-	-3	w8
		- 00 11000 - 44- 0 - 0		0.397	-	
923.095746	4241424.0	$C_{61}H_{77}N_{14}O_{33}P_5S_5$	923.096179	0.469	-2	b6 - B(T) - 2H
967.902837	4151589.1					

968.044500 968.333185 978.621335 986.765884 986.909570 987.050642 987.192503 987.341248 987.484432 987.624034 987.768381 987.910174 988.052659 988.194762 988.338898	3734020.7 3043272.2 3440072.3 5960020.0 8953948.3 17746801.1 13556670.8 26739502.1 23429293.1 14436886.9 16992280.7 13805289.2 12029292.8 4052850.4 3481989.4					
988.483293 990.476305	3825607.2 3320268.7	C ₁₅₇ H ₂₀₀ N ₄₁ O ₈₄ P ₁₅ S ¹⁵	988.482997	- 0.299	-5	M - 5H - H2O - 3G
990.624617	3067207.2					
992.757896	3719915.1 3783891.7	C126H161N44O66P12S	1024.34508	-	-4	w12 + 1H
7	010000111	12	6	0.128	·	
1052.30329	5622486.1	C ₁₆₇ H ₂₁₁ N ₅₁ O ₈₇ P ₁₅ S	1052.30330	0.018	-5	M - 5H - 4H - G
0 1052.50399 9	7405075.9	15	9			
1052.70279	7833578.0					
5 1052.90432 0	5294575.1					
1055.90183	3100235.0					
0 1075.11011 2	3267878.0	$C_{71}H_{90}N_{16}O_{38}P_6S_6$	1075.11031 9	0.193	-2	b7 - B(G) - H2O
1075.86346	3326007.0					
2 1076.36278 9	3645160.8					
1082.31257 0	10466432.4	$C_{172}H_{215}N_{56}O_{88}P_{15}S$	1082.31162 6	- 0.872	-5	M - 7H
1082.61548 5	3083246.9					
1082.91254 4	36286291.5					
1083.01772 1	3002794.0					
1083.11384 7	36452864.1					
1083.31513 6	17896598.9					
1083.42104 0	3103759.3					
1083.51612 5	21661937.4					
- 1083.71724 0	12776943.2					
1083.91509 8	10887387.2					
1084.11236 1	4803423.8					

1084.31283	5945151.7					
, 1087.71303	5082201.7					
1087.90614	4270487.7					
1088.10762 3	3107436.5	$C_{71}H_{88}N_{18}O_{38}P_6S_6$	1088.10556 8	- 1.889	-2	b7 - B(T) - NH3, b7 - B(dC) - H2O
1091.30841 6	3665822.8					
1136.13729	3295350.0	$C_{36}H_{46}N_{13}O_{18}P_3S_3$	1136.13860 0	1.147	-1	w3
, 1151.56176	3741146.2		0			
1151.72959	6737100.1					
5 1151.89402	17000089.1					
2 1152.06150	18328471.2					
1 1152.23362	5446595.1					
7 1152.38953	8271059.4					
0 1152.72524	3471172.8					
4 1353.89064	5310646.4					
2 1354.13580 8	6076402.0					
1354.38901 2	4319268.8					
1354.63958 9	4682717.7					
1355.14018	5207944.7					
1382.47698	3860447.3					
5 1382.67222	6238887.5					
1382.86852	6115882.6					
o 1861.93905 0	3760599.8					
			Abs mean error	0.959		
			Abs mean std dev	0.630		

Table S17 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of eight scans accumulated denoised (sane rank 10) [M-8H]⁸⁻ precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured	Intensity	Elemental	Theoretical	Error	Charg	Assignme
mz	-	Composition	mz	(ppm	e	nt
)		
225.438894	11759881.8					
225.480452	20634793.2					
225.522342	22940480.3					
225.560402	15049862.9					
225.564129	30139274.8					
225.606010	31214371.5					
225.647282	15226010.1					
225.689377	11952232.0					
255.829077	19316912.4					
255.866098	23910769.7					
255.903160	25059992.8					
255.940238	24048392.3					
255.977294	1/413053.6					
256.014316	13404631.2					
257.694575	12111649.4					
257.742248	24770340.7					
257.789898	2/8448/2./					
257.832177	11282582.8					
257.837472	30063962.0					
257.879829	10832184.7					
257.885183	26087329.1					
257.932820	18189140.3					
287.809916	12224024.4					
287.851524	19088202.0					
287.893375	23352918.3					
287.935039	23404561.1					
287.976749	18066402.6					
288.018354	12791091.4					
300.757856	12114244.0					
300.813040	148/0000./					
300.869299	1415/3/3.4					
300.925009	11930000.1					
338.149141	10712040.1					
338.13/003	87490000.8					
330.211932	20313000.0					
330.220417	179430009.1					
330.229914	2010000.Z					
000.214002 228 282016	42402133.3 230275050 2					
JJU.Z02940 338 780055	208210008.0					
220 202440	12030329.4					
330.292419	29902000.0					
229 245227	19000334.0					
330.343227	123907 109.9					
338 300557	25423334 6					
338 408134	136304/51 1					
338 /176/0	16033750 5					
338 462118	23211803.7					
338 4705/1	164508807 3					
338 /8012/	1800/252 7					
338 524710	18800334 1					
338.532957	116778531 4					

338 542190	13894130 8					
338 595473	50540979 9					
338 658052	22870862.8					
338 720632	28422035.2					
338 783508	10705351 5					
330 531323	10858874 0					
330 656003	15055020.8					
220 710521	1090000.0					
220 702072	22420011.3					
339.102013	19030334.9					
339.043003	11417300.0					
345.410177	11203000.2					
345.405023	10/9335/.8					
383.085380	147 10390.0					
383.741213	17070903.4					
383.796586	17608415.3					
383.852286	24222443.1					
383.907967	24/11214.2					
383.963316	16825734.4					
386.610815	19282546.1					
386.682605	26562856.6					
386.753211	24873864.5					
386.825391	27988552.3					
386.897146	13175529.8					
386.968469	14930597.8					
387.039541	11078221.4					
431.709955	15912016.4					
431.772121	17833350.7					
431.898385	17286147.8					
431.960695	16153512.0					
432.023703	16884895.7					
432.086242	12546612.9					
451.047579	13153659.7					
451.215157	16094341.2					
451.298468	10755289.6					
451.381117	15957339.9					
451.465164	14513489.1					
493.528031	12893472.7					
493.599935	11644258.1					
493.671163	12400816.6					
541.153697	12374991.5					
541.355479	10756654.8					
601.062029	14595940.1					
601.171233	25327542.0					
601.282872	40403789.2					
601.394917	92949580.8					
601.506636	82231459.5					
601.617600	58733483.0					
601.728632	52108203.6					
601.839887	31549002.7					
601.949923	22619237.6					
602.172615	12713756.9					
603.948997	14164293.4					
604.059083	13391735.6					
605.500416	14636254.1					
609.559319	13537658.8	$C_{76}H_{99}N_{25}O_{40}P_7S_7$	609.559960	1.052	-4	w7 + 1H
609.809664	10899912.7					
627.666897	11054005.1					
627.849803	24703999.1					
628.032160	15285161.7					
628,122443	20155409.5					

628.211554 657.594107 657.814485 657.939406 658.096570	15632809.5 16071412.9 13297545.3 11246564.8 19999589.3	$C_{46}H_{57}N_{12}O_{22}P_3S_3$	658.096992	0.641	-2	a4 - 2H, b4 - H2O
659.438772 659.564405 659.689051 659.814158 659.939718 660.064439 660.190322 660.315540 674.322732	15934196.6 31480666.9 56689889.6 71027739.8 38934465.7 30666402.6 17446197.9 12373038.4 58835771.6					
674.426800 674.447992 674.573359 674.663555 674.698183 674.785443 674.798655 674.823262 674.910511 674.948469 675.037127 675.073201 675.197719 675.323510 675.448337 675.573971 675.695040 675.895646 676.065715 676.075682 676.092080 676.100429 676.100429 676.110337 676.118526 676.128294 676.136328 676.154486 676.163228 676.154486 676.163228 676.171489 676.182074 676.200437 676.224569 676.243095 676.243095 676.243095	19389511.2 126915113.7 223545789.8 12075475.4 243971952.9 13397877.6 10617579.7 238662689.2 13483108.4 198142699.3 11218940.4 140015943.5 99927066.2 62319977.8 41352931.9 20435996.4 13328474.6 11420838.4 13189434.3 12308493.9 10842609.9 11111300.4 11349554.3 12715203.9 12116991.3 13168017.5 13258734.0 14586209.5 13046430.0 15235822.9 16363957.0 20054946.6 21674916.1 20947177.6 21557275.7 27540640.5 25811434.0 43927533.2	C ₆₆ H ₈₅ N ₂₃ O ₃₂ P ₅ S ₅	674.426811	0.016	-3	y6 + 1H
676.271067 676.284199	57832387.5 266512846.3					
676.319538	3711907137.0	$C_{172}H_{217}N_{56}O_{88}P_{15}S$	676.318994	0.804	-8	M - 8H
676.344221	122748138.1	19				
070.357581 676.364999	105215032.7 86789533.3					
676.377036	93934400.6					

676.384853	118898764.8
676.394530	139707029.2
676.409694	681588094.7
676.445016	8946301569.0
676.468470	313852942.8
676.479144	227731385.2
676.486099	222884341.3
676.495918	1/5606497.7
6/6.50/0/5	180599524.6
070.034011	1100705827.0
0/0.5/0285	14380099779.
676 501560	U 511561112 2
676 603100	311301143.3
676 610830	350900330.0
676 620157	276203500 0
676 620850	261070230.0
676 638203	272598834 7
676 659515	1304192660 0
676 695440	17367096566
070.000440	n
676 726580	353435851.9
676 735440	411562048 5
676 744341	308235577 6
676,754013	277297230.9
676 762469	295354426 1
676 784195	1201765070 0
676.820452	15681695238.
0101010101	0
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676.868327	260396222.5
676.878288	226356326.1
676.886846	247095927.5
676.897894	261595134.5
676.908859	942932701.8
676.922612	390204927.6
676.945455	11780666661.
	0
676.984792	246655934.5
677.002517	154393241.2
677.011312	170076783.2
677.021109	180209311.3
677.033985	664340382.2
677.046859	281418317.0
677.070428	8134591761.0
677.094059	233801278.3
677.109566	160945079.8
677.136844	125694943.2
677.144908	110006933.3
677.158949	455099725.8
677.171020	182582823.0
677.040044	53284/3/13.0
o//.219211	172919024.3
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0/1.259646	00092000.0
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011.203904	212001440.5 107250227 0
677 220477	101300321.9
011.020411	5220139209.0
011.330310	00409941.0

677.361785	62646460.9				
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677.389604	36580606.4				
677.408965	154163562.6				
677.422944	75908193.5				
677 445660	1864000626.0				
677 468202	63876438 1				
677 / 80807	37/66371 6				
677 400007	20001500 7				
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677.506891	22988654.2				
677.523063	41734965.4				
677.536474	55327023.7				
677.544742	35182583.7				
677.570750	1004292209.0				
677.605407	21451896.3				
677.612047	25253645.6				
677.624463	29162445.6				
677.635066	32143943.7				
677.658773	27185132.0				
677.670561	21100586.1				
677.695757	508171581.0				
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677.735862	22667412.9				
677.745075	11447705.9				
677,754819	11147948.8				
677 783352	25030779 3				
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677 820548	272107067.6				
677 856666	37500108.6		677 857/33	1 1 3 2	-5 c10
077.000000	57590100.0	C106I 1134I N33 C56F 10	011.001400	1.152	-0 010
677 009060	12010201 7	10			
677.004095	12940201.7				
677.045700	1104/020.0				
077.943790	130307702.4				
678.054865	2/482/65.4				
678.071362	68274249.5				
678.196496	40678460.0				
678.257760	22100285.6				
678.320804	31551900.7				
678.444724	38127797.1				
678.461484	13748390.7				
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679.109895	32356576.1				
679.115862	30150081.3				
679.136317	15111139.4				
679 156502	75507154 7				
679 192894	1121813027 0				
679 233607	30738420 3				
670 2/2628	23875010 /				
670 2512/0	2160//0/ 2				
670 261040	21004404.3				
019.201010	016/0600 6				
	21643683.6				
679.281731	21643683.6 104481654.8				
679.281731 679.318004	21643683.6 104481654.8 1551603804.0				

679.358896	37228438.4
679.367644	30116232.8
679.377614	25943381.7
679.386449	26152981.1
679.406588	116181943.1
679.443111	1665021285.0
679.477068	29503998.8
679.484400	40143350.2
679.492913	28943202.0
679.502865	25981848.1
679.512120	25165927.8
679.531512	101597466.4
679.568159	1454425778.0
679.590065	52408377.6
679.603188	25677605.1
679.609115	35138598.6
679.621090	22555202.2
679.637228	20783647.9
679.656553	76154575.9
679.693064	1065668903.0
679.716039	36186730.5
679.734039	22374825.1
679.743518	15822832.5
679.754435	12409352.5
679.767175	12649881.1
679.781435	49003125.6
679.792399	20871344.3
679.818020	708900705.2
679.856743	13389746.4
679.906228	28847986.7
679.919178	12229698.3
679.942976	408325173.6
680.031053	13233507.7
680.067943	220644153.7
680.193143	123681833.8
680.317936	61615172.0
680.443133	31140700.6
680.567642	13393086.8
680.695638	10529179.8
681.062511	65960806.0
681.188086	148978038.0
681.277277	14089977.3
681.313049	181916727.0
681.402808	16046823.2
681.438250	163797937.3
681.527091	11746415.9
681.563568	159464226.1
681.655196	14862742.7
681.688237	121524792.4
681.813069	79257822.0
681.938496	60774134.5
682.063365	44962694.0
682.189190	30739064.1
682.315078	17995287.0
682.393571	11842820.2
682.441055	13083775.1
682.562024	17503484.3
682.728178	12759628.7
689.239118	16368977.8
690.434825	11744994.7

690.534668 690.634684	32984040.6 71673669 2					
690 698291	14692772 1					
690 734291	107736935.6					
690 798875	15918413.3					
690 835456	140156056 1					
690 896913	13256806.4					
690 933217	71607449.0					
691 034986	56522436.9					
691 135091	60528765.5					
691 236486	29588016.3					
691 336755	24719777 6					
691,437744	12941558.8					
691.536513	11385122.5					
692.732939	11331566.9					
693.034607	13171241.5					
693.234360	12545221.7					
727.874134	11470268.4					
728.076194	10994359.4		728.075556	-	-3	b7 - B(dA) +
		071. 93. 100 40. 000		0.876	•	1H 🦾
743,330883	20099105.9		743.329984	-	-4	a9 - 2H, b9 -
		• 90· · 119· · 31 • 40· · 8 • 8		1.209	·	H2O
743.581969	18751672.4					
743.831196	14154047.8					
747.403952	10525565.7					
747.571049	14093538.6	$C_{51}H_{61}N_{10}O_{27}P_4S_4$	747.569771	-	-2	a5 - B(dC) -
				1.710		NH3
747.739094	14147142.8					
751.788679	10522301.3					
752.479474	10795332.2					
752.700694	11319363.1					
754.071483	12832265.7					
754.361293	16764074.2					
754.504564	20615324.8					
756.234557	11248140.2					
765.820788	13216401.4					
765.928777	15265388.8					
766.754813	21400666.4	$C_{76}H_{95}N_{21}O_{39}P_6S_6$	766.754257	-	-3	a7 - 2H, b7 -
				0.725		H2O
767.090072	25679505.9					
767.328480	10870517.4					
767.374060	95589773.4					
767.421659	22242280.7					
767.441890	20584379.3					
767.485528	170532977.5					
767.553228	16827398.5					
767.595889	203220826.8					
767.661685	21401555.9					
767.706556	194829219.4					
767.760032	12644328.9					
767.771620	12862505.9					
767.817120	119023306.8					
767.880746	11726289.3					
767.927148	72998483.9					
767.993652	16624008.9					
768.041224	127453290.2					
768.154166	65256243.5					
768.264819	57959751.5					
768.375062	58846487.3					
768.482947	14854398.6					

769.927028	22566059.5					
770.039040	55332377.4					
770.151122	27761336.5					
770.260115	27381435.4					
770.371894	23922016.1					
770.481477	11952994.3					
770.705026	12655137.3					
770.943865	11937421.5					
771.085485	14104429.4					
771.811723	11100856.5					
772.937302	19553552.6					
773.081377	83841335.2					
773.179428	23110321.9					
773.221892	114279276.9					
773.319835	37879631.6	C96H120N35O48P0S0	773.321472	2.117	-4	w9 - H2O
773.365251	208624448.9	- 30: 120: 33 - 40: 3 - 3				
773,461746	46286790.2					
773 508565	200306047.2					
773 609642	23828721 6					
773 654269	327312237 0					
773 686418	11190123.8					
773 751538	14201239.8					
773 795456	144616478.8					
773 939885	116487333 7					
774 080739	82800964 4					
774 223056	53876855 3					
774.225950	25057307 1					
774.500455	13631332.2					
776 221013	23871/72.0					
776 262902	16221016 /					
776 509105	2/2022/010.4					
776 651110	262001546					
776 702057	20021107.0					
776 025706	2961/729 2					
777 070897	20014730.2					
777.079007	31440013.1					
777 26/92/	20090024.0					
770 644004	10172004.0					
770 700605	20140040.4					
770 024422	20230340.3					
770.931123	13009299.0					
779.074077	21310011.0					
779.217340	13310409.8					
779.301339	10122213.0					
779.501722	11942039.0					
779.788329	11122074.5		704 477745		F	a12 2∐ b12
791.478732	31005382.4	$C_{126}H_{157}N_{40}O_{65}P_{11}S$	/91.4///45	-	-5	H2O
704 070000	202000000	11		1.247		
791.679388	39306896.2		704 000075	4 000	~	a10
791.879582	41998413.0	$C_{126}H_{159}N_{40}O_{65}P_{11}S$	791.880875	1.633	-5	alz
700 000000	04500400 4	11				
792.080093	31520186.4					
/92.280796	1/1/7177.6					
809.246303	16644133.9					
809.412342	23216125.3					
809.579503	19044517.5					
809.746416	16467742.3	a a a				-
812.747574	12870647.3	$C_{76}H_{98}N_{25}O_{40}P_7S_7$	812.746430	-	-3	W/
			0.10.100-0	1.408		
818.107316	16011662.3	$C_{56}H_{70}N_{14}O_{28}P_4S_4$	818.108589	1.556	-2	a5 - 2H, b5 - H2O
819,275073	52596087 8		819,275150	0.094	-5	a13 - B(G) -
310.210010	02000001.0	- 130 · 100 · 38 · 68 · 120	510.210100	0.007	~	(⁻ /

		40				OCH2
819.475355	64369570.3	$C_{126}H_{162}N_{44}O_{66}P_{12}S$	819.476178	1.004	-5	w12 + 2H
		120 102 11 00 12				
819.675503	47806977.1					
819.876282	17703045.9					
823.837336	13942329.4					
840.345743	11777147.7	$C_{106}H_{134}N_{40}O_{52}P_9S_9$	840.347617	2.230	-4	y10 + 1H
846.915599	12597742.3					
847.039170	15354322.8					
860.488881	69397072.9		000 00007	0.000	-	-12
800.089231	81249951.9	$C_{136}\Pi_{172}N_{46}O_{69}P_{12}S$	800.090007	0.902	-D	215
861 090208	34738544 0	12				
861 290736	14139747 8					
861 549009	14333955.6					
861.670962	11743795.8					
861.798485	12390528.4					
861.923809	13691754.1					
862.047268	15417829.2					
862.173728	18705763.6					
863.295052	48621105.1					
863.422678	67101568.7					
863.546842	149716915.4					
863.613880	17506733.7					
863.671945	198630692.7					
863.738329	26302576.3					
803.790472	160819029.4					
003.003499 863.020402	1947 1000.7					
863 088252	1005/082.2					
864 046350	133101730 6					
864 113713	15242110 1					
864.171555	123970255.3					
864.297026	84985989.4					
864.423167	51105170.6					
864.545709	16347984.5					
864.796836	11574765.8					
866.170126	11205622.0					
866.293670	13299150.7					
866.419250	36824019.5					
866.542522	19828941.7					
866.667197	29689839.7					
800.794007	21501471.5					
867 044321	14027900.0					
868 164424	11102665.6					
876 751483	17414368.2					
876.919118	23027610.7					
877.085663	21365685.1					
877.252823	21270245.0					
877.419610	13403425.6					
879.585372	13079132.7	$C_{55}H_{70}N_{18}O_{29}P_5S_5$	879.585111	-	-2	w5 - CH3
				0.297		
879.751081	14340136.5					
880.254453	12233948.4					
881.250354	1282/221.0					
881.419977	15443818.8					
001./01200	2219/194.0					
002.099030 880 121707	24102012.9		883 136033	1 /01	-3	a8
002.434191	10003044.1	<u>086111091126</u> 044 F 707	002.400000	1.401	-0	40

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884.775025	18390093.1					
885.106853	15700664.7				-	_
887.097234	18021759.8	$C_{56}H_{73}N_{18}O_{29}P_5S_5$	887.096848	-	-2	W5
				0.435		
899.597965	13288820.7					
899.765799	15149942.2					
901.695091	11478893.7					
901.759553	122778873.3					
901.862887	24223042.1					
901.898376	12002471.4					
901.926704	303927230.3					
901.958898	13331222.1					
902.029647	37200899.8					
902.093255	400320716.2	$C_{61}H_{77}N_{11}O_{33}P_5S_5$	902.091568	-	-2	a6 - B(dA) -
				1.870		H2O
902.124231	19917386.3					
902.196690	44944276.3					
902.260192	376572874.8					
902.306329	11322104.3					
902.362648	48543755.7					
902.427629	397904510.0					
902.471546	12349761.9					
902.529871	22798121.4					
902.699833	16372616.5					
902.762951	232565056.8					
902.868574	15362958.7					
902.927711	100337238.1					
903.093095	74022499.9					
903.261488	48022782.5					
903 430430	32397493.9					
903 595352	17466982 6					
903 763802	17404714 2					
905 422936	10755858.9					
905 590564	25794471 1					
905 757559	32705607.4					
905 923863	32808430.6					
906 258433	36141482 7					
906 424145	24764250 2					
906 592660	24704200.2		906 593201	0 597	-4	b11 - OCH2
000.002000	21020270.1		000.000201	0.007	•	
906,756599	12987119.9	i U				
908 420432	13396279 1					
908 586620	14270513 7					
908.751229	15828301 7					
908 921424	16875758 2					
909 088063	11416212 5		909 089280	1 349	-4	a11 - 4H
000.000000	11710212.0	U10 142 38 59 100	000.000200	1.0-10	т	
922 426338	14966400 4		922 424684	-	-3	w8
022.420000	14000400.4		022.424004	1 793	U	
958 472703	10977358 2					
985 197706	12217350.2					
985 343104	123167124					
986 764560	14788277 2					
086 01010/	70640366 5					
087 05/272	95871028 5					
087 107582	80831172 0					
087 765507	100004413.2					
901.200001 087 22000F	10929000.4 63630060 1					
301.JJ32JJ 007 100001	03032000.1 52571050 1					
901.402U01	55574050.1 56152500.0					
901.025826	0.06020100					

987.766926 987.909402 988.051253 988.197215 990.196256 990.333454 990.481376 990.623133	33654666.8 28935358.3 17882166.5 14403989.7 12650624.9 11899469.8 27181195.8 18573180.6					
1082.71481 6	30309872.0	C ₁₇₂ H ₂₁₇ N ₅₆ O ₈₈ P ₁₅ S	1082.71475 6	- 0.055	-5	M - 5H
1082.91480 6	29851596.4					
1083.11400 2	73156029.5					
1083.31189 9	57383994.4					
1083.51598 0	47861205.6					
1083.71480 4	31053941.0					
1083.91663 1	30976967.3					
1084.11454 1	20420216.0	$C_{71}H_{92}N_{16}O_{39}P_6S_6$	1084.11560 2	0.979	-2	b7 - B(G), a7 - B(dA) + 1H
, 1084.31146 7	13569367.1		Z			
, 1084.51742	13212094.5					
1087.31027	16784253.0					
4 1087.50901	11913049.3					
1087.71136	12913778.6					
1087.90910	12245671.9					
1088.11240	23228179.9					
o 1136.13382	10712712.6					
3 1151.39408	12282233.0					
8 1151.55945	14788016.2					
9 1151.72944	22131812.5					
8 1151.89597	45249656.7					
2 1152.06142	39570943.3					
1152.22705	41326302.8					
9 1152.39537	19584780.9					
9 1152.56279	27995687.2					
1152.72959	15200096.2					
o 1155.72491	16103813.3					

1					
1155.89114 7	14244689.0				
, 1156.05951	11956896.0				
6	40005747.0				
1353.63948 5	10985717.6				
1353.88871 3	25053416.2				
1354.13887 8	17623126.5				
1354.38815 3	20485819.9				
1354.63878 1	18375871.6				
1354.89130 6	25336053.4				
1355.13874 5	12319478.2				
1359.63527 7	17646862.6				
1359.88404 7	13157710.4				
1360.13300 1	12078421.2				
1382.87431 3	12593353.7				
1383.07090 1	16593731.3				
1861.93930 5	19587310.2				
		Ab	s mean	1.137	
		err	or		
		 Ab std	s mean I dev	0.583	

Table S18 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of eight scans accumulated denoised (sane rank 10) [M-7H]⁷⁻ precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured	Intensity	Elemental	Theoretical	Error	Charg	Assignme
mz	•	Composition	mz	(ppm	e	nt
)		
257.838424	20418300.2					
257.885993	18954883.9					
338.345496	19843117.6					
383.906832	17600333.8					
383.962441	23400248.7					
386.539385	46162125.0					
386.599523	22250355.7					
386.610572	81275075.9					
386.671224	33975331.3					
386.682332	152304949.3					
386.694558	17824673.3					
386.742680	40383695.2					
386.753884	222242482.6					
386.766051	26371694.0					
386.814040	40791443.1					
386.825362	182379635.2					
386.837682	19728741.3					
386.885086	22547274.7					
386.896645	112698181.3					
386.968167	43485391.9					
387.039690	65234864.7					
387.111155	66467387.3					
387.182570	43044557.6					
387.254056	19100942.7					
388.180853	23779861.4					
388.323988	26649484.9					
388.395359	32599042.5					
388.466915	22129958.6					
601.061295	31577605.1					
601.172952	114693357.9					
601.285123	83567964.7					
601.395328	145168596.6					
601.507292	79735865.3					
601.617696	25533326.8					
601.728672	47559978.1					
601.840651	43133191.5					
603.837275	16066612.9					
604.059850	20520937.3					
627.758825	22279152.6					
627.850963	24471178.4					
627.941962	17386690.8					
628.122600	20869765.0					
674.697369	17550213.6					
674.823429	17912579.6					
676.321314	79012197.0					
676.410989	35410569.1					
676.445753	92452409.2					
6/6.535907	49281608.9					
676.572636	147917752.5					
676.660289	51212116.8					
6/6.695032	213841477.9					
676.785779	40760860.4					

676.821787	287855330.4
676.912797	21624964.5
676.945880	170107020.9
677.036868	19217923.2
677.071898	132467033.7
677.197315	59124758.5
677.319022	48462359.2
677 447704	37223692.8
677 572394	21789816.6
670 103883	28785367.4
670 318553	20700007.4
670 444020	29004029.4
670 560507	29091905.1
670,602597	10010409.1
079.093080	31/08/45.0
679.819332	29049859.7
681.189870	16791443.8
681.313407	22896832.8
681.688943	19386241.3
681.938815	18842291.8
690.535961	43624701.0
690.636556	83275014.2
690.699427	21430985.5
690.736041	75731415.5
690.799510	17070488.5
690.836818	73494187.1
690.937792	89589300.8
691.037592	76356158.9
691 137367	47377160 7
691 235957	30343871.0
751 788701	17120/00 1
752 500800	15950605 1
752 799/12	54524207.0
753.700413	106047011 4
753.931944	120047911.4
754.074721	100701402.2
754.217835	132/04510.1
754.361130	/1340888.0
754.504178	38134998.5
754.646501	30718001.5
754.789436	15828765.5
765.708789	22267989.4
765.821042	16547398.0
765.934030	23303124.7
767.217714	20525266.4
767.258496	99362653.6
767.327912	52466042.6
767.371602	357468581.6
767.397075	18152165.3
767,419807	24598081.7
767 439221	80232210 7
767 483055	749962300 4
767 508062	32131068 1
767 528633	38830308.8
767 540520	20033330.0 85380607 1
767 504064	1000560477 0
101.394301	1000009177.0
101.03/124	49040090.2
101.000005	106296754.2
/6/.705341	1082796598.0
767.747291	52776343.2
767.771345	90095053.4
767.816579	960070601.5

767.856742	44495703.9					
767.883971	88660842.0					
767.927772	788764229.5					
767.966171	34527683.9					
767.995776	64621649.5					
768.039155	566678711.3					
768.076524	32487673.9					
768.150080	382110409.4					
768,186855	21528595.2					
768.220888	28612327.1					
768 261914	259293766 0					
768 298431	15835215.3					
768 322467	16705306.3					
768 331194	18402795.4					
768 372608	1/0880050 2					
768 /8/070	11/17500/ 3					
762 702262	10494160 9					
769 707340	10704065 0					
762 210/10	204903.9					
700.019419	20409727.1					
700.940090	20/00/20.0					
760 945240	00090220.0 150600610 5					
769.015310	10000010.0					
769.879990	22/89302.8					
769.926686	282690849.4					
769.950099	15827633.2					
769.992229	30032759.7					
770.017016	16821452.4					
770.037968	424580442.4				_	
770.059563	26214864.7	C ₇₁ H ₉₀ N ₂₃ O ₃₈ P ₇ S ₇	770.060238	0.877	-3	w7 - B(T) - 2H
770.103788	33385802.1					
770.149176	440233127.6					
770.180263	16591603.4					
770.193013	16600459.8					
770.214809	29256824.8					
770.260575	426549810.8					
770.283284	22457631.3					
770.325708	24689915.3					
770.349309	17876809.8					
770.371681	408008645.0					
770.393095	24202076.2					
770.405740	17169564.7					
770.430634	19527805.9					
770.482989	303684770.0					
770.594096	224630913.7					
770.705359	156802280.2					
770.813931	78921762.7					
770.924730	55692369.1					
770.942873	130269623.9					
771.036929	38313377.2					
771.084510	196398584.4					
771 149822	15950313 8					
771 182905	19341915 4					
771 227435	227707500 9					
771 264105	17749815 7					
771 328237	18258530 5					
771 370525	254576102 6					
771 472611	22613322					
771 512521	22010022.0					
771 580656	77628701 /					
771.000000	11020131.4					
//1 6560//						

771.700673 771.744728 771.755524 771.797329 771.813374 771.840420 771.870804 771.890060 771.923109 771.968257 771.984785 772.005905 772.033960 772.083538 772.116412	147330760.2 20805394.8 21301228.7 104568613.1 192461369.1 17538519.3 21912765.8 17735157.1 230840423.3 17359032.3 23816533.4 17634835.2 236975603.9 73170961.9 16504288.6					
772.145104	213382488.2					
772 257137	171946766 4					
772.323129	24292717.9	$C_{96}H_{124}N_{31}O_{51}P_9S_9$	772.322409	- 0.932	-4	d9 + 2H
772.368214	181968522.5					
772.416628	26187707.5					
772 479647	138475133 4					
772.548597	15881323.5					
772.592172	106110657.3					
772.662820	17524560.8					
772.675378	15893467.3					
772 721707	20686678 6					
772.733195	19000890.0					
772.761746	37202500.8					
772.780108	21233263.9					
772.816531	67114025.9					
772.837050	24173604.4					
772 860888	24030302.1					
772.886943	24686811.9					
772.913185	33035282.6					
772.931194	42205925.6					
772.944082	41352566.3					
772.953165	38/8041/.8					
772.975488	39502920.3					
773.001209	64043153.6					
773.013450	67348590.9					
773.033820	338419726.7					
773.080678	4334640920.0	C ₁₇₂ H ₂₁₇ N ₅₆ O ₈₈ P ₁₅ S	773.079889	1.021	-7	M - 7H
773 122035	143228451 8	15				
773.134550	162580579.6					
773.145046	154854387.3					
773.157826	190312316.0					
773.177031	834897457.7					
773.223861	10074010261.					
773 255057	375664185 1					
773.268236	273777491.0					
773.278956	295359946.8					
773.290526	275122752.8					

773.366887 1585	56668303.
0	00000 5
773.386826 9312	262990.5
773.399014 4300	000204.9
773.417899 3540	J/4853.2
773.441335 3010	043741.4
773.463095 1374	4813013.0
773.510113 1744	4916642.
772 551501 2023	772047 0
772 662200 4620	23047.0
	203101.2
772 605740 4243	001903.0
773.610390 6204	
772 652960 1560	144913.0
113.052600 1500 0	J7 562 125.
772 69/276 5120	066025.0
772 609/20 2172	200923.0
773 709000 3039	220370.3
773 710870 2047	719779 0
772 747450 0124	126244 7
772 705907 112/	13620261
113.193001 112 ² 0	+3000001.
773 8/83/7 2583	811655 0
773 858310 2106	S95564 4
773 800313 667/	11/017 7
773 00/252 3308	221/7/ /
773 038756 7060	075218 0
773 067000 2810	07108 1
773 082382 1686	S/1523 Q
773 003178 1033	2014/1323.9
774 004723 1500	01441.3
774 033608 4433	317673 1
774.050606 4450	177322 2
77/ 081/52 5080	7777308 N
77/ 113218 1/8/	183708 0
774 133276 1172	202640 4
77/ 1/0280 6763	202040.4
774 176001 2848	206373 0
774 224531 3107	7999612.0
774 277340 7757	73069 4
774 289472 561	50794 3
774 302350 4937	74040 4
774 319241 1727	704444 1
774 336788 7207	75043 1
774 367116 1889	0863539.0
774 399112 5290	05034 7
774 421701 3384	16975 0
774 434935 249	5793 7
774 464062 9414	16099 7
774 510377 1053	8690591 0
774 563540 2134	18859 5
774.583682 3989	90352.0
774.605171 4282	29536 1
774 653161 6027	765010 2
	00010.0
774.686327 2302	21836.7
774.686327 2302 774.703082 2621	21836.7 18119.6
774.686327 2302 774.703082 2621 774.746668 4429	21836.7 18119.6 53526.0
774.686327 2302 774.703082 262 774.746668 4425 774.796146 3125	21836.7 18119.6 53526.0 534314.6

774.886091	16743757.2
774.939835	154624208.3
775.082930	124919379.9
775.104968	22484866.1
775.224358	47908280.4
775.249363	42033908.0
775.345035	24812042.5
775 364710	44293535.2
775 414407	33766669 3
775 507936	47870275 3
775 580764	22201703 7
775 650772	50404077 9
775 600061	09494077.0
775.003201	200/0201.3
775.747700	10240522.5
775.794144	60170795.9
//5.85189/	25224095.5
775.938176	55795808.2
776.081931	52227287.4
776.173374	61278723.7
776.198458	30330097.6
776.221086	763181671.2
776.253707	24669608.2
776.273830	35132560.0
776.284256	28174854.1
776.296644	31652893.4
776.316874	128582026.2
776 364297	1715108008.0
776 394608	68077512.8
776 /08/65	45680506 A
776 420403	43009300.4
776 420107	44033321.2
770.430074	40447014.0
776.459565	185342447.5
776.507164	2448/133/2.0
776.559310	63354165.5
776.571419	56288525.7
776.583067	46967412.0
776.602267	186418839.9
776.616355	97724307.4
776.650015	2561250836.0
776.681098	88120679.1
776.703849	53881439.4
776.717754	48525776.1
776.744746	174225560.2
776.793065	2247368425.0
776.835395	43172039.2
776 846254	56242318.8
776 857967	45624050 5
776 8709/8	40024000.0
776 887500	132731027.0
776 004922	62160522.0
776.025716	1695624174.0
770.935710	1085034174.0
1/0.90/550	50032312.8
//6.98/65/	35862624.0
///.009675	26891128.6
777.030223	91954246.4
777.043129	44204536.2
777.078818	1156090529.0
777.108350	41398196.8
777.124149	21215022.1
777.132922	26427182.9

777.145144	21374786.9					
777.172898	58770226.1					
777.221693	717384032.2					
777.275010	17552765.9					
777.315722	32066784.5					
777.364339	397523312.9					
777.458580	17394664.9					
777.507511	207164678.8					
777.650338	106624908.5					
777.793601	54793831.3					
777.936525	33981801.5					
778.079709	31275593.0					
778.501752	183436533.6					
778.579742	26625210.0					
778.591975	27301723.6					
778.644881	373923185.1					
778.745850	66681019.6					
778.788034	480816821.1					
778.883586	37547448.0					
778.930920	526394417.8					
778.953624	23929056.2					
778.983537	17082831.0					
779.026015	32327647.2					
779.073715	437755261.4					
779.169126	23001843.8					
779.216293	294135353.8					
779.236879	35778409.8					
779.312352	16340064.1					
779.359344	218888488.9					
779.419078	18203144.4					
779.502341	165631735.0					
779.576213	15857164.7					
779.645521	123937370.4					
779.789226	93930025.4					
779.932579	65900060.4					
780.075893	47745062.2					
780.219252	36846721.3					
781.926606	16334942.8					
818,107523	19570031.6		818,108589	1.303	-2	a5 - 2H, b5 -
		- 30: 70: 14 - 20: 4 - 4			_	H2O
819.275617	17113993.2	C ₁₃₀ H ₁₆₅ N ₃₈ O ₆₈ P ₁₂ S	819.275150	-	-5	a13 - B(G) -
		12		0.570		UCHZ
819.474627	24544927.2	C ₁₂₆ H ₁₆₂ N ₄₄ O ₆₆ P ₁₂ S	819.476178	1.893	-5	w12 + 2H
		12				
823.337198	18992478.1	$C_{106}H_{132}N_{33}O_{54}P_9S_9$	823.335782	-	-4	b10 - H2O,
				1.720		a10 - 2H
823.587193	21435512.6					
823.836964	16417339.9					
846.790968	16112235.2					
847.041412	22849771.6					
858.078070	20938921.2					
858.245256	26422512.1					
858.412626	24927683.3					
861.547175	15858404.2					
861.673564	17225979.7					
861.799307	22114962.4					
861.925084	16604723.6					
863.295211	50952106.3					
863.364804	17840397.9					
863.420738	69886690.7					
863.489259	28934006.5					

863.546419 863.614566 863.671535	122452002.6 38663979.9 143488494.6					
863 738500	3/20820/ 0					
863 703287	15/67/530 0					
863 864536	31532378 0					
863 022018	151752257 0.8					
003.922910	101702204.0					
003.992730	22002011.2 141777560 4					
004.040700	141///002.4					
004.110000	20331907.1					
004.173045	105902307.0					
004.297991	100010001.1 50412201.0					
004.4227 10 964 546540	21700461 7					
004.040040 966.400206	31700401.7					
866 546060	31441029.4 12217071 7					
866 660855	30510000 1					
866 703002	24247010 4					
200.793902 221 /22022	24247019.4					
001.420923	27230049.9		001 764150	0 124	2	b8 - H2O - a8 -
001.704032	57110070.0	U86H107N26U44F737	001.704150	0.134	-3	2H
882.097217	28425847.0					
882.432957	19704412.5					
887.097359	36084433.9	C ₅₆ H ₇₃ N ₁₈ O ₂₉ P ₅ S ₅	887.096848	-	-2	w5
				0.576		
887.598445	16180782.7					
901.928236	21684067.3					
902.096213	65093486.1					
902.263695	99978697.4					
902.367849	23153881.9					
902.432081	108638662.8					
902.535011	22324207.3					
902.598612	102453879.3					
902.700301	28507464.3					
902.764430	135600532.4					
902.865082	18739315.5					
902.932167	105250922.8					
903.097389	119320691.1					
903.264784	74129212.0					
903.430814	64305415.2					
905.925285	1//13/9/.1					
906.094511	39192167.6					
906.261629	2/11/15/.4					
906.427004	31863699.9					
906.760884	18/83521.5		000 500004	0.005	4	o11 0U b11
909.593124	23412234.1	$C_{116}H_{144}N_{38}O_{59}P_{10}S$	909.593201	0.085	-4	H2O
000 944504	10221211 1	10				
909.844591	19331341.4		000 404604		2	w/8
922.420315	32302037.3	U86H110N30U44P838	922.424004	-	-3	WO
022 750401	35513950 /		022 760626	1.700	2	w8 + 1H
922.739491	26388830.2	0861 1111 1 30044F 808	922.700020	1.230	-5	
925.092557	20300030.2					
900.77 1021 986 016104	261807826					
086 076153	173/56/27					
987 055052	72554222					
987 1200/2	10360422 3					
987 198655	80198894 4					
987 264402	20758398 7					
987 341002	85851847.9					
987.409105	18284303.3		987.408586	-	-3	w9 - B(A) -
		00 114-00-49.9-9			-	

				0.526		CH3
987.483500 987.625555 987.769387 987.912541 988.051056 988.198285 990.194575 990.338315	92245507.3 88094319.6 99113910.6 71220573.4 27068137.1 18729768.9 20789868.6 24212408.3					
1024.34426 6	26254518.9	C ₁₂₆ H ₁₆₁ N ₄₄ O ₆₆ P ₁₂ S	1024.34508 6	0.801	-4	w12 + 1H
1052.10036 0	18575587.5	$C_{65}H_{82}N_{23}O_{34}P_6S_6$	1052.09994 9	- 0.391	-2	w6 - CH3
1052.50243	63754996.3		-			
3 1052.70213 7	62212497.5					
י 1052.90275 9	47153161.2					
1053.10411 2	24012500.2					
1053.30439	22885735.3					
o 1055.50185 5	15967392.9	C ₁₆₇ H ₂₁₁ N ₅₁ O ₈₈ P ₁₅ S	1055.50229	0.414	-5	M - 5H - 4H - dA
1055.70028	23732066.8	15	Z			
9 1055.90133	21568506.8					
1075.60960	18965405.2	C ₁₃₆ H ₁₇₀ N ₄₆ O ₆₉ P ₁₂ S	1075.61041 5	0.754	-4	z13 - 2H, y13 - H2O
1075.86103	22088284.9	12	0			
3 1076.11071	34414699.3					
1076.36119	19712292.2					
9 1082.31041	84874754.0	$C_{172}H_{215}N_{56}O_{88}P_{15}S$	1082.31162	1.121	-5	M - 7H
3 1082.61918 0	25567295.2	15	0			
1082.71116	293698963.9					
5 1082.81970	29496334.1					
1082.91113	265927766.4					
4 1083.01843	28700199.2					
0 1083.11222 8	219096346.6					
1083.21682	21447401.0					
7 1083.31516 7	154579955.9					
, 1083.51607 2	126934842.1					
∠ 1083.71816	60674057.8					
- 1083.91537	42354647.1					

16941790.0 22132995.9 26749605.9 28565442.8 26472335.7 24068795.8 20624595.1 16811857.2 17253307.6 24183287.2	C ₁₃₁ H ₁₇₀ N ₃₈ O ₇₀ P ₁₂ S 12	1382.47308 7	- 0.140	-3	b13 - B(G) + 2Н
16941790.0 22132995.9 26749605.9 28565442.8 26472335.7 24068795.8 20624595.1 16811857.2 17253307.6	C ₁₃₁ H ₁₇₀ N ₃₈ O ₇₀ P ₁₂ S	1382.47308	- 0.140	-3	b13 - B(G) + 2Н
16941790.0 22132995.9 26749605.9 28565442.8 26472335.7 24068795.8 20624595.1 16811857.2					
16941790.0 22132995.9 26749605.9 28565442.8 26472335.7 24068795.8 20624595.1					
16941790.0 22132995.9 26749605.9 28565442.8 26472335.7 24068795.8					
16941790.0 22132995.9 26749605.9 28565442.8 26472335.7					
16941790.0 22132995.9 26749605.9 28565442.8					
16941790.0 22132995.9 26749605.9					
16941790.0 22132995.9					
16941790.0					
18048895.3					
26845493.4					
37813837.5					
47493622.9					
52253253.1					
23466870.9					
29780909.2		0			
21014505.2	$C_{36}H_{46}N_{13}O_{18}P_3S_3$	1136.13860	2.455	-1	w3
17665523.0					
17318814.4					
29356786.5					
36003920.7					
24385286.1					
20289929.3					
22801339.6					
20921223.6					
29659549.7					
	29659549.7 20921223.6 22801339.6 20289929.3 24385286.1 36003920.7 29356786.5 17318814.4 17665523.0 21014505.2 29780909.2 23466870.9 52253253.1 47493622.9 37813837.5 26845493.4 18048895.3	29659549.7 20921223.6 22801339.6 20289929.3 24385286.1 36003920.7 29356786.5 17318814.4 17665523.0 21014505.2 23466870.9 52253253.1 47493622.9 37813837.5 26845493.4 18048895.3	29659549.7 20921223.6 22801339.6 20289929.3 24385286.1 36003920.7 29356786.5 17318814.4 17665523.0 21014505.2 21014505.2 23466870.9 52253253.1 47493622.9 37813837.5 26845493.4 18048895.3	29659549.7 20921223.6 22801339.6 20289929.3 24385286.1 36003920.7 29356786.5 17318814.4 17665523.0 21014505.2 23466870.9 52253253.1 47493622.9 37813837.5 26845493.4 18048895.3	29659549.7 20921223.6 22801339.6 20289929.3 24385286.1 36003920.7 29356786.5 17318814.4 17665523.0 21014505.2 C ₃₆ H ₄₆ N ₁₃ O ₁₈ P ₃ S ₃ <u>1136.13860</u> 2.455 -1 0 23466870.9 52253253.1 47493622.9 37813837.5 26845493.4 18048895.3

Table S19 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of eight scans accumulated and no denoising of [M-8H]⁸⁻ precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured	Intensity	Elemental	Theoretical	Error	Charg	Assignme
mz		Composition	mz	(ppm	е	nt
000 405550	0000500 0)		
200.425558	6283539.9					
200.402841	0020001.4					
225.438893	10564576.9					
225.476471	8765118.5					
225.480420	20235333.8					
223.318172	7412878.0					
225.522299	21003522.4					
225.559900	9072240.0					
225.500042	11120083.0					
225.503882	24188506.1					
225.001777	5331210.5					
225.000030	29049693.2					
225.643932	6298006.9					
223.047212	14118482.3					
225.689457	10128796.4					
230.210639	6809572.8					
230.244376	0903408.3					
230.277589	0843291.7					
230.311181	0504221.7					
200.791807	9150258.4					
255.828731	13964739.8					
255.866139	20940972.7					
255.897366	5413032.3					
255.898092	5370569.2					
255.903066	22720304.8					
255.940279	23383738.8					
200.977210	10022604.0					
200.014402	10900094.0					
200.001422	01/0323.0					
257.094434	9700704.0					
257.730907	20042680 0					
257.7942072	20943000.9					
257 780770	24402470 2					
257,709770	24492470.3					
257.052050	26957695 5					
257.057401	20037003.3					
257.079001	0007900.1					
257.000291	15526221 5					
257.332073	7007820 8					
257.900337	6167080 5					
230.020323	11200606 3					
207.009933	17235836 1					
207.031290	20522761 2					
207.033030	6526855 8					
201.021120	200330/6 7					
207.00000	16204621 /					
288 018365	11478101 3					
288 050033	8007202 1					
288 101617	56317/0 5					
300 757844	10864341 1					
300.813637	14085221.6					

300.869185	13089753.2
300.924915	10196626.9
300.979957	7313086.5
301.035630	5361555.0
329.023385	8831407.2
329.071255	8974949.8
329.118858	8761442.4
329,166318	6757794.4
329 214359	6336887.0
338 148919	9996115.4
338 157618	860507864
338 166037	0357618 2
338 21108/	23300/55 1
228 220281	177/0/085 7
220 227104	12102072 /
220 220007	74002756 6
330.229001	24902750.0
330.203311	00007400 F
338.274441	40837490.5
338.282972	238611139.4
338.288848	10/9814/.6
338.292424	29318420.6
338.328669	6391733.2
338.336519	16268964.8
338.345279	117302715.8
338.354877	12837458.9
338.399620	23633136.4
338.408128	131695057.9
338.417500	14667035.1
338.457906	5496055.0
338.462611	20814561.9
338.470569	163063350.6
338,480093	18049850.3
338.524765	16055415.2
338.533045	115202339.5
338 542252	12997218 8
338 587176	6452986 8
338 595476	49465456 7
338 605597	6696162.2
338 658021	21080000 7
338 720672	2601003/6
338 783535	1036/205 7
338 844803	6010677 0
220 521560	10020710.0
220 504462	9420740 5
339.39440Z	0439749.3
339.000739	14203734.1
339.7 19408	20814921.2
339.782124	18199472.0
339.843707	9182199.9
361.113056	5/6/694.0
383.685358	5352942.9
386.969608	/9/2403.8
431.769954	6341798.1
431.772778	6472232.0
450.963783	7264978.4
451.048442	10696618.4
451.382093	10076517.8
451.463471	5652740.5
493.530118	7702541.5
493.671806	6680951.7
609.309896	11550987.1

609.559242 609.810216	9216438.5 7808747.2	$C_{76}H_{99}N_{25}O_{40}P_7S_7$	609.559960	1.178	-4	w7 + 1H
651.744645	9225509.9	$C_{66}H_{83}N_{16}O_{34}P_5S_5$	651.744365	- 0.430	-3	a6 - 2H, b6 - H2O
657.564527	5743051.6					
657.595375	14006995.2					
657.814236	12567703.7					
657.938688	9221949.9			4 9 5 9	•	
658.096299	15484725.9	$C_{46}H_{57}N_{12}O_{22}P_3S_3$	658.096992	1.053	-2	a4 - 2H, 04 - H2O
658.192303	5537026.2					
650 564205	14037009.4					
650 688005	55570588.8					
659 781251	5890799 1					
659.814191	70581335.3					
659.939619	38193419.4					
660.064381	28268046.5					
660.190927	14735174.3					
660.317239	8068170.7					
662.438245	7356643.8					
662.560593	7694032.5					
673.699843	5609723.2					
673.820911	5050401.9					
673 045478	8402406 5					
674 071544	5450020.8					
674.089927	13901930.3	C66H84N23O32P5S5	674.090870	1.399	-3	y6
674.322631	57370597.1	- 00: 04: 23 - 32: 3 - 3			-	-
674.447981	125660984.7					
674.538726	10000074.7					
674.573342	222532358.1					
674.605544	6006663.7					
674.612821	6112957.9					
674.632176	6209525.6					
674.662890	12500210.5					
674.090150	6032350 1					
674 785529	14146881 1					
674.799090	10050048.1					
674.823208	236531015.8					
674.847057	8402166.4					
674.864656	6385417.0					
674.910776	13490518.5					
674.924748	6602609.0					
674.948454	196619717.5					
675 036060	5395263.7 11444742.0					
675 052909	6083351 2					
675 073115	136537023 5					
675.093744	7509758.8					
675.164049	7498853.9					
675.197688	97864741.5					
675.292823	6026325.4					
675.323435	60621294.0					
675.354785	5495965.5					
b/5.448433	40240666.9					
010.019134	0000121.0 10/10015 2					
675 620/06	6262650 1					
675.650416	6054593.2					

675.725929 727862.7 675.74610 6625046.3 675.781449 5917186.7 675.80366 5462040.0 675.813663 9515328.9 675.803668 5773140.8 675.8346449 533317.9 675.8346449 533317.9 675.895760 10740931.1 675.895760 10740931.1 675.895760 10740931.1 675.895760 10740931.1 675.997951 6993720.3 675.997951 6993720.3 675.996080 7142499.9 675.996080 7142499.9 675.996080 7142499.9 675.996080 7142499.9 675.996080 7142499.9 675.996080 7142499.9 675.996080 7142499.9 675.996080 7142499.9 675.996080 7142499.9 676.01338 7945611.4 676.01338 7945611.4 676.01338 7745611.4 676.01338 7745611.4 676.01338 7745611.4 676.01338 7745611.4 676.01338 7945611.4 676.016302 12245651.8 676.036302 12245651.8 676.036302 12245651.8 676.036302 12245651.8 676.103631 118070 1249148.3 676.10871 10242459.9 676.103631 118070 12491458.5 676.103631 12893707.7 676.125201 11804627.3 676.103631 12893707.9 676.11541 1034627.3 676.103631 12893707.9 676.136331 12893707.9 676.136331 12893707.9 676.16271 12829779.9 676.16271 12829779.9 676.	675.694376	12480324.5					
675.7749610 6622046.3 675.77649 5917186.7 675.786051 662040.0 675.80513 6074806.0 675.818630 9515328.9 675.834668 5773140.8 675.844494 5334317.9 675.845449 5334317.9 675.865393 6756735.1 675.897361 0246938.4 675.920726 7381225.0 675.931816 10246538.4 675.947418 9433826.0 675.966952 734525.0 675.97849 17881420.6 675.9685431 8524541.4 676.014338 7945611.4 676.014338 7945611.4 676.014338 794561.4 676.014338 794561.4 676.014338 794561.4 676.016911 8127329.6 676.049277 9558692.4 676.049277 9558692.4 676.049277 9558692.4 676.049277 955869.4 11804414.3 676.075894 11804414.3 676.01389 1104183.2 676.101384 11034627.3 676.101384 11283070.7 676.145538 13175443.8 676.154305 14177985.9 676.12491458.5 676.12491479.9 676.674.7218 216.6397.7 676.445538 13175443.8 676.634558 21116880.7 676.24473 216.16397.5 676.24473 216.16397.5 676.24473 216.16397.5 676.24473 216.16397.5 676.24473 216.16397.5 676.24473 216.16397.5 676.24473 216.16397.5 676.34558 137.5447.20.5 676.34558 211.16880.7 676.24473 216.16397.5 676.34558 211.16880.7 676.24473 216.16397.5 676.34558 211.16880.7 676.24473 216.16397.5 676.345581 317.5443.8 676.345581 317.5443.8 676.345591 345.5 676.345681 345.5475.9 676.345681 345.5475.9 676.345681 345.5475.9 676.345681 345.5475.9 676.345681 345.5475.9 676.344571 345.5475.9 676.344571 345.5576.0 676.344571 345.5576.0	675.725929	7278682.7					
67.7, 78449 591 / 186./ 675.7, 800513 6074806.0 675.816030 9515328.9 675.816030 5737140.8 675.84648 5737140.8 675.846449 5334317.9 675.846449 5334317.9 675.847516 6993720.3 675.847516 6993720.3 675.847516 6993720.3 675.847516 6993720.3 675.847516 6993720.3 675.847616 6993720.3 675.847616 6993720.3 675.931816 10246538.4 675.947918 9433826.0 675.966952 7346501.8 675.9678491 784420.6 675.978491 784420.6 676.014393 9110422.0 676.014391 8127329.6 676.014393 9110422.0 676.014393 9110422.0 676.014393 9110422.0 676.014393 9110422.0 676.014593 11249458.5 676.104501 11249458.5 676.104502 12245651.8 676.110154 11034627.3	675.749610	6625046.3					
07.5.80001 0402440.0 075.800051 60748005.0 075.830466 577.3410.8 075.83766 6993720.3 075.87366 6993720.3 075.83766 6993720.3 075.83766 6993720.3 075.876761 6993720.3 075.876761 6993720.3 075.87267 7381275.0 075.973618 9433826.0 075.9737819 9433826.0 075.9737819 7681420.6 075.973781 852541.4 076.00303 9110422.0 076.00303 9110422.0 076.014338 7945611.4 076.014338 7945611.4 076.014338 794561.4 076.014937 1082485.9 076.01737 1082485.9 076.01737 1082485.9 076.11670 12491485.5 076.11670 12491485.5 076.11670 12491485.5 076.11670 12491485.5 076.12674 103382.2 076.12674 12491485.5 076.126747 1039032.2	675.778449	5917186.7					
0712000315 00740000 0758.81630 9515328.9 0758.834668 5773140.8 0758.84648 5334317.9 075.847449 5334317.9 075.847649 010740931.1 075.85760 10740931.1 075.85760 10740931.1 075.85760 10740931.1 075.937816 9433826.0 075.937816 9433826.0 075.937817 9433826.0 075.967867 742499.9 075.937849 9433826.0 075.937847 8524541.4 076.01438 8524541.4 076.01338 5794571 076.01338 579454.4 076.01438 8524541.4 076.003043 9110422.0 076.00303 91542.6 076.01438 8524541.4 076.003038 7945611.4 076.003038 91542.6 076.10429 958692.4 076.00339 1104183.2 076.10439 11024627.3 076.104391 11024627.3 076.145381 13175443.8 <	675.780051	6462040.0					
0712010030 501320.3 07583408 5773140.8 07583408 5773140.8 075845130 6993720.3 07583516 6993720.3 07583516 6993720.3 07583516 6993720.3 07583516 6993720.3 07594756 6993720.3 075947518 9433826.0 07594718 9433826.0 07594718 9433826.0 07594718 9433826.0 07594718 9433826.0 075956952 7346501.8 07500030 71142499.9 075105694718 8524541.4 07600303 9110422.0 076013339 9751354.4 07600303 1924559.9 07600302 12245651.8 0760075694 11004414.3 076101051 10241485.5 076101051 11034627.3 076101051 1417995.9 076102639 1289370.7 0761128207 1995069.6 076120440 21430644.5 07624473 1289575.9 076161371	075.000513 675.919630	0074000.0					
07:10:00:00 07:17:10 07:5:844:44 5334:317.9 07:5:87:87:61 6993720.3 07:5:87:87:61 6993720.3 07:5:87:87:61 6993720.3 07:5:87:87:61 10240538.4 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 7142499.9 07:5:90:80 714449.4 07:0:00:303 9110422.0 07:0:00:303 9751354.4 07:0:00:303 9751354.4 07:0:00:303 11041433.2 07:0:01:303 11041433.2 07:0:10:30382 11041433.2 07:0:11:40:0 11951089.6 07:1:16:70 12941458.5 07:1:16:20 11951089.6 07:1:16:20 1114860.7 07:1:22:11116800.7	675 834668	57731/0.8					
675.865393 6756755.1 675.865393 6756755.1 675.885760 10740931.1 675.89576 10246538.4 675.99718 10246538.4 675.99718 10246538.4 675.997319 9433826.0 675.997319 9433826.0 675.997319 9433826.0 675.997319 9433826.0 675.997319 943826.0 675.997320 7345601.8 675.9978491 7681420.6 676.013033 7914521.4 676.013338 7945611.4 676.014338 7945611.4 676.014338 7945611.4 676.014338 7945611.4 676.016302 12245651.8 676.016302 12245651.8 676.110154 11034627.3 676.118670 147143458.5 676.118670 14177985.9 676.118671 128975.9 676.118671 128975.9 676.214291 12894583.3 676.22473 21616397.5 676.23779 26204517.4 676.22473 21616397.5 <td>675 848449</td> <td>5334317 0</td> <td></td> <td></td> <td></td> <td></td> <td></td>	675 848449	5334317 0					
675.875016 6903720.3 675.875016 10740931.1 675.895760 10740931.1 675.92072 7381275.0 675.947181 9433826.0 675.947181 9433826.0 675.947181 9433826.0 675.947181 9433826.0 675.947181 9433826.0 675.98680 7142499.9 675.986803 9104122.0 676.003043 9104122.0 676.01333 7945611.4 676.01333 97451354.4 676.01333 9751354.4 676.053939 9751354.4 676.063039 91104183.2 676.01339 91104183.2 676.110154 11034627.3 676.110154 11034627.3 676.110154 11034627.3 676.110154 11034627.3 676.110154 11034627.3 676.110154 11034627.3 676.110154 11034627.3 676.110154 11034627.3 676.11128 112893707.7 676.11128 13175443.8 676.22003 11118180.4 </td <td>675 865393</td> <td>6756735 1</td> <td></td> <td></td> <td></td> <td></td> <td></td>	675 865393	6756735 1					
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	675.978491	7681420.6					
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010.03639 9731334.4 676.046927 9558692.4 676.066302 12245651.8 676.075894 11804414.3 676.0775894 11804414.3 676.0773 10824859.9 676.100839 11041833.2 676.110154 11034627.3 676.118670 12491458.5 676.138391 12893707.7 676.145338 13175443.8 676.154305 14177985.9 676.163771 12829779.9 676.163771 12829779.9 676.163771 12829779.9 676.163771 12829779.9 676.171431 14954588.3 676.206440 20141186.0 676.206440 20141186.0 676.206440 21430644.5 676.20633 24106847.5 676.22473 21616397.5 676.234203 27503131.8 676.243079 26204517.4 676.243079 26204517.4 676.2624175 268050987.1 676.365178 6936364.8 676.365178 6936364.8 676.365178 6936364.8 676.37010 94011437.8 676.384861 118879772.2 676.344241 122742875.8 676.347549 105487206.1 676.365178 6936364.8 676.37010 94011437.8 676.384861 118879772.2 676.344501 189542016.0 676.445011 8954261760.0 676.445011 8954261760.0 676.445011 8954261760.0 676.445013 222857652.6 676.446103 222857652.6 676.446103 222857652.6 676.446103 222857652.6 676.446103 222857652.6 676.446103 222857652.6 676.44501 322857652.6 676.44501 322857652.6 676.446103 222857652.6 676.44501 322857652.6 676.44501 322857652.6 676.44501 322857652.6 676.44501 322857652.6 676.446103 222857652.6 676.44501 322857652.6 676.44501 32457653 31 676.44501 322857652.6 676.44501 322857652.6 676.44501 32457653 31 676.44501 322857652.6 676.44501 322857652.6 676.44501 322857652.6 676.44501 32457653 31 676.44501 322857652.6 676.44501 322857652.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.44501 32457752.6 676.4751357775777777777777777777777777777777	070.010911 676 022920	0751251 4					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	676 046027	9751554.4					
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	676 075894	11804414.3					
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.100839	11041833.2					
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$\begin{array}{cccccccccccccccccccccccccccccccccccc$	676.154305	14177985.9					
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	676 224472	21110000.7					
$ \begin{array}{c} 676.243079 \\ 676.243079 \\ 26204517.4 \\ 676.260339 \\ 44000645.4 \\ 676.271087 \\ 57941805.8 \\ 676.284175 \\ 268050987.1 \\ 676.319520 \\ 3711390056.0 \\ C_{172}H_{217}N_{56}O_{88}P_{15}S \\ 676.318994 \\ 0.778 \\ -8 \\ M \\ -8H \\ \end{array} \right) \\ \begin{array}{c} 15 \\ 15 \\ 676.344241 \\ 122742875.8 \\ 676.357549 \\ 105487206.1 \\ 676.365117 \\ 86936364.8 \\ 676.377010 \\ 94011437.8 \\ 676.384861 \\ 118879772.2 \\ 676.394535 \\ 139547018.0 \\ 676.409713 \\ 684000758.1 \\ 676.445011 \\ 8954261760.0 \\ 676.468475 \\ 313950146.2 \\ 676.479138 \\ 22857652.6 \\ 676.495905 \\ 175403236 \\ 3 \\ \end{array} \right) $	676 23/203	27503131.8					
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	676 495905	175403236 3					

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679 883324	8957084 0
679 892971	6486607.8
670 0061/7	2036/5/5 0
670 010206	11166204 6
670 042007	11100204.0
670 002472	400437041.0
670,000064	1122911.0
679.990064	0230009.3
080.000190	5841154.1
680.018541	6695175.3
680.031417	13249843.9
680.067981	218560746.9
680.123883	5471049.6
680.156362	7522427.0
680.176140	5980645.0
680.193094	121835296.2
680.209376	7794365.7
680.317918	60812421.1
680.443168	29945405.2
680.567734	12810985.8
680.695264	9470752.2
681.028774	5385960.5
681.062484	66401964.2
681,152437	9173855.1
681,187912	147773019.0
681.277232	12723385.8
681.312905	177802561.8
681 329928	7847968 1
681,403325	14875185.6

681.438155	159690318.1					
681.457022	8216506.4					
681.527707	8892202.5					
681.563403	144222874.0					
681.656144	9986318.8					
681.688346	106437895.1					
681.704897	7115469.0					
681,812794	73384331.3					
681 937548	52777004 1					
682 063506	40734526.0					
682 189023	27615023.3					
682 314498	15792067.4					
682 393667	11371508 7					
682 440207	10650373.8					
682 561340	15005652 1					
682 727340	11758538 7					
682 805621	9710210 6					
600 524144	12160516 5					
600 622217	13100310.3					
090.033217	22228087.0					
090.732100	20110322.9					
690.795078	5354786.4					
690.832070	52216398.1					
690.897282	6782820.2					
690.932856	35260976.4					
691.033791	23330967.5					
691.066093	6068146.5					
691.130161	15327810.7					
691.233932	10508235.0					
691.265306	6110901.3	C ₁₀₆ H ₁₃₅ N ₄₀ O ₅₄ P ₁₀ S	691.265336	0.043	-5	w10 + 1H
		10				
691.335777	6219438.8					
727.084806	6556542.8	$C_{46}H_{60}N_{16}O_{23}P_4S_4$	727.085251	0.612	-2	w4
727.873346	9172761.5					
735.638899	5803970.0					
735.783714	5832423.5					
743.079983	7376810.7					
743.330605	19127765.4	$C_{96}H_{119}N_{31}O_{48}P_8S_8$	743.329984	-	-4	a9 - 2H, b9 -
				0.835		H2O
743.581269	17119895.9					
743.831480	12537551.3					
747.405274	6486820.0					
747.571234	12183073.9	$C_{51}H_{61}N_{10}O_{27}P_4S_4$	747.569771	-	-2	a5 - B(dC) -
		01 01 10 21 1 1		1.957		NH3
747.740528	12216790.4					
756.234292	7082383.6					
766.754484	14895610.4	C76H95N21O39P6S6	766.754257	-	-3	a7 - 2H, b7 -
		-70. 35. 21 - 55. 0 - 0		0.296	-	H2O
767.090639	23153471.6					
767 421282	18944377 2					
767 706835	8001143 3					
767 817845	6946879 4					
767 929163	7294697 3					
768 029243	7273050 9					
768 040284	5636748 6					
770 02640	14066700 5					
770 2538/0	5020122 2					
772 027222	17705766 6					
772 2021 002	5508251 4					
113.223449	1200204.4					
772 506404	10001000.0					
113.506481	10423160.8					

773.651522 773.786355 773.795281 773.932829 774.070193 776.220645	9144505.4 5437728.2 6152600.4 5453761.2 8635289.7 7567384.4					
778.325844	6771042.9					
791.277064	6226487.4					
791.478748	28754417.4	$C_{126}H_{157}N_{40}O_{65}P_{11}S$	791.477745	-	-5	a12 - 2H, b12 - H2O
791.679354	36897129.9	11		1.207		
792.079746	30438966.8					
792.281366	13491149.7					
809.077764	5841456.5					
809.246136	15890250.6					
809.412196	22815707.5					
809.579732	18316372.6					
809.746787	15766667.4					
809.914779	6771103.0					
810.077140	5501691.1					
812.748202	9202391.3	$C_{76}H_{98}N_{25}O_{40}P_7S_7$	812.746430	- 2 180	-3	w7
819 074612	28569824 2		819 073048	2.100	-5	w12
010.074012	20000024.2		010.070040	1 909	-0	
819 220415	5550435.0	12		1.000		
819.274962	52290415.6	C120H165N20O60P12S	819,275150	0.229	-5	a13 - B(G) -
		12			-	OCH2
819.422534	7184155.3	12				
819.475402	63904557.3	C ₁₂₆ H ₁₆₂ N ₄₄ O ₆₆ P ₁₂ S	819.476178	0.947	-5	w12 + 2H
		12				
819.675886	45571726.5					
819.875976	15412186.9					
820.077956	6560619.1					
823.833035	5957543.9					
823.841855	6588368.4					
830.623490	5342580.2					
840.091565	7931207.1					
840.599579	8270514.0	$C_{106}H_{135}N_{40}O_{52}P_9S_9$	840.599573	-	-4	y10 + 2H
860.430327	6262493.1			0.007		
860.488880	68891577.9					
860.628366	6829201.6					
860.689167	80972890.8	C136H172N46O69P12S	860.690007	0.976	-5	z13
		12				
860.829987	5879001.0					
861.089337	33395271.1					
861.288047	5519519.4					
876.751391	17358765.2					
876.918929	22152213.7					
877.085231	20495767.9					
877.254409	15467859.3					
879.419195	8041107.1					
879.584874	9788439.6	$C_{55}H_{70}N_{18}O_{29}P_5S_5$	879.585111	0.269	-2	w5 - CH3
879.745011	9173166.0					
879.755507	7048694.5					
880.254828	8824063.2					
881.074885	6058578.9	$C_{81}H_{104}N_{27}O_{43}P_8S_8$	881.074322	-	-3	w8 - B(dC) + 1H
881 244901	6804232 5			0.039		
881.420759	9691362.0					
	-					

881.761144 882.098561 884.441931	15091422.2 13568270.9 7133534.2	$C_{86}H_{107}N_{30}O_{41}P_7S_7$	884.440000	-	-3	y8 - H2O, z8 - 2H
884.775315 885.105826 887.097153	16006561.0 14242401.0 10786752.6	C56H73N18O29P5S5	887.096848	-	-2	w5
899.591610 899.601609 899.769160 901.694883 901.733126 901.759657 901.792118 901.862961 901.899268 901.926663 901.958861 901.999395	6861310.8 6400823.9 9292505.9 11287003.1 7728151.7 122586861.5 5810678.1 24235777.8 11855159.2 304344436.3 12865685.8 5380859.0	- 30. 13. 118 - 23. 3 - 3		0.344		
902.029453 902.092961	35997212.2 390071901.9	$C_{61}H_{77}N_{11}O_{33}P_5S_5$	902.091568	- 1.544	-2	a6 - B(dA) - H2O
902.124964 902.163434 902.191293 902.254325 902.290769 902.356759 902.425455 902.763958 905.423023 905.590447 905.751326 905.761813 905.920954 908.417144 909.842076 910.345379	19214649.9 5823013.7 28783024.9 263406086.6 14367056.8 30776969.3 219862424.5 13620831.1 8408437.1 24573790.6 14933553.4 14971105.5 9045567.5 5446119.8 5626306.0 6355825.2					
922.426427	10344271.6	$C_{86}H_{110}N_{30}O_{44}P_8S_8$	922.424684	- 1.890	-3	w8
1000.35978 4 1000.86009	5485614.4 5657582.0	C ₁₂₆ H ₁₆₀ N ₄₄ O ₆₄ P ₁₁ S ¹¹	1000.35921 4	- 0.570	-4	y12 + 1H
5 1015.98131	5457066.3					
1 1861.96204 3	6261963.2					
Ŭ			Abs mean error Abs mean	0.975 0.678		
			std dev	0.010		
Table S20 showing peak list, intensity, elemental composition, and possible assignments with mass errors (ppm) of danvatirsen using 2D-UVPD-MS of eight scans accumulated and no denoising of [M-7H]7- precursor ion (note, noise peaks were included to highlight the effect of denoising).

Measured <i>mz</i>	Intensity	Elemental Composition	Theoretical <i>mz</i>	Error (ppm	Charg e	Assignme nt
)		
257.880350	8656641.1					
257.885623	20971989.3					
319.013154	8923661.9	$C_{41}H_{52}N_6O_{25}P_4S_4$	319.013110	- 0 138	-4	d4 - B(dA) - NH3
383.685016	16832640.0			0.100		
383.739782	18728249.9					
383.796832	30384586.8					
383.841274	11083282.4					
383.852797	48936345.1					
383.862631	9043590.6					
383.897121	14116631.4					
383.908148	75367695.8					
383.919355	12916776.0					
383.952884	12169487.7					
383.963527	78840005.0					
383.973789	9065037.8					
384.008457	10094076.3		204 040405		-	6 P(T) 4U
384.019236	44266219.5	$C_{61}H_{75}N_{14}O_{34}P_6S_6$	384.019125	-	-5	CO - D(T) - 4H
384 063865	7/00762 /			0.209		
384 074677	2/501650 1					
384 130362	13692752.2					
385 073607	10669592.1					
385 129184	14020356.3					
385 184926	12929334 0					
385.240197	8553282.4					
385.469652	7420791.5					
385.541151	11781058.6					
385.612926	10526686.3					
385.684355	11057577.9					
386.528174	9132113.4					
386.539149	66769154.5					
386.551490	7725611.1					
386.599373	19763618.2					
386.610730	75757626.7					
386.623652	9309687.3					
386.671337	23824795.5					
386.682138	1/8660383./					
386.694210	19753646.6					
386.742571	35468281.5					
300.733030	208033307.8					
300.703044	20079120.3					
300.014330	24034091.0					
386 837024	22/20827 5					
386 885373	14947688 9					
386 896552	94644305 7					
386 908615	11403562 6					
386,956956	7347168.5					
386,968370	32278126.9					
387.039433	56892624.4					
387.052119	6797378.6					

387.111064	51447387.3
387.182483	28916837.5
387.253943	11582320.6
388.394884	7563984.9
541.458285	9123272.1
601.176134	9232661.6
601.290031	8412681.5
601.393193	7698256.9
601.402285	24294772.3
601.513525	16352078.2
609.307192	6932970.0
657.593610	8644245.0
676.322540	28892183.2
676.415897	10264339.6
676.451893	27299838.5
676.540136	22448912.7
676.573497	18500462.2
676.579689	36090250.2
676.669898	10885601.6
676.691761	20682934.0
676.700843	30917891.9
676.817986	13903403.9
676.828797	31893400.7
676.942318	7514385.9
676.949219	66563168.5
677.072658	17401257.7
677.198238	8486095.9
679.197871	15938168.1
679.695238	9614949.2
679.821528	8549446.7
690.530828	14405421.7
690.540087	18368713.7
690.642822	12683531.1
690.706187	7351357.8
690.734446	11356248.6
690.845418	7916596.3
691.041177	6929355.7
691.235037	7281356.5
727.579960	9328618.0
751.646966	10703373.8
751.788451	14384390.2
751.931246	13300777.6
752.481725	8039227.1
753.147415	8592686.1
753.788483	62697771.1
753.884982	11313664.5
753.931808	123156530.6
753.951465	7616655.3
754.028362	15691990.3
754.074546	160005013.5
754.094943	9178387.0
754.171932	13365368.3
754.217743	112702701.5
754.312992	8050238.6
754.361566	71742531.7
754.505553	21920359.3
754.643711	13223443.8
755.499481	10063223.2
755.645306	7051220.6
756.075737	6768089.5

 $C_{76}H_{98}N_{25}O_{40}P_7S_7$

609.308004 1.333 -4 w7

1.985 2 ⁴¹ 765.707875 48017151.3 7<
fbb.70076 48017151.3 765.750766 7664844.7 765.820125 75035043.0 765.827867 7443041.6 765.827867 7437041.6 765.8278687 7437041.6 765.8278687 7437041.6 765.93240 84104951.2 766.076834 7650789.0 766.13954 9107772.8 766.171854 9107772.8 766.207469 7384172.0 766.202491 9312248.7 766.202491 9312248.7 766.316365 756553.6 766.316365 756553.6 766.316365 756553.6 766.428863 9766740.7 766.428863 9766740.7 766.441624 6986114.6 766.428863 9766740.7 766.441624 6986114.6 766.428863 9766740.7 766.441624 6986114.6 766.428863 9766740.7 766.41263 8374147.2 766.428863 9766740.7 766.41263 837447.2 766.41263 936814.6
765.30700 765.320125 75035043.0 765.820125 75035043.0 765.820387 7144588.2 765.878587 7437041.6 765.893996 7886030.1 765.893986 84104951.2 766.04258 72864709.7 766.07883 7650789.0 766.113954 9107772.8 766.171674 7325082.6 766.242412 9312248.7 766.233351 7506562.5 766.316365 756553.6 766.41283 8374147.2 766.42863 9766740.7 766.42863 9766740.7 766.43620 778964.5 766.45620 778964.5 766.45620 778964.5 766.45620 778964.5 766.45620 778964.5 766.45620 778964.5 766.45620 778964.5 766.45620 778964.5 766.45620 778964.5 766.57467 7314461.5 766.57467 7314461.5 766.57467 7314461.5 766.683357 77456228.4
705.2012.0 7144588.2 765.878587 7437041.6 765.878587 7437041.6 765.8392480 84104951.2 766.07683 72864709.7 766.07683 72864709.7 766.113954 9107772.8 766.113954 9107772.8 766.1143954 9107772.8 766.20499 7384172.0 766.23351 7506562.5 766.338951 7506562.5 766.338951 766533.6 766.412633 8374147.2 766.422863 9766740.7 766.412633 8374147.2 766.428863 9766740.7 766.41624 6968114.6 766.454620 7778964.5 766.514688 7566258.4 766.535818 7766018.4 766.5357 72103.6.8 766.63357 8274032.5 766.63357 8274032.5 766.6631357 925426.5 766.63357 82703.8 766.63357 82703.8 766.73657 721036.8 766.76365 14580612.4 <t< td=""></t<>
103.03.03 1443.041.6 765.878587 7437041.6 765.878580 84104951.2 766.042858 72864709.7 766.076834 7650789.0 766.13954 9107772.8 766.171674 7325082.6 766.207469 7384172.0 766.207469 7384172.0 766.207469 7384172.0 766.20351 7506562.5 766.316365 7865533.6 766.316365 7865533.6 766.412833 8374147.2 766.42863 9766740.7 766.441624 6968114.6 766.436035 25474524.5 766.514888 7566258.4 766.535818 7766018.4 766.633367 721036.8 766.633367 721036.8 766.633367 721036.8 766.78108 1405591.5 766.78108 1405591.5 766.782839 10044179.1 766.782355 14380632.7 766.78108 14045591.5 766.78108 14045591.5 766.782355 14380631.1 <t< td=""></t<>
105.05.05 7886030.1 765.93240 84104951.2 766.04258 72864709.7 766.113954 910777.8 766.113954 910777.8 766.171674 7325082.6 766.224749 7384172.0 766.23351 7506562.5 766.33635 7665533.6 766.33635 7665533.6 766.41623 8374147.2 766.424803 9766740.7 766.42863 9766740.7 766.42863 9766740.7 766.41624 696114.6 766.53365 7566258.4 766.53465 7566258.4 766.53457 7314461.5 766.63357 827036.8 766.63357 827036.8 766.63357 827036.8 766.683357 827036.8 766.68229 9229190.5 766.783457 7314461.5 766.683357 827036.8 766.68229 9229190.5 766.783457 7314461.5 766.783457 7314461.5 766.783459 10044179.1 766.7834
105.03030 84104951.2 766.042858 72864709.7 766.042858 72864709.7 766.113954 9107772.8 766.17147 7325082.6 766.207469 7384172.0 766.224912 9312248.7 766.3316365 7565533.6 766.316365 7565533.6 766.316365 7565533.6 766.412633 8374147.2 766.42863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766740.7 766.43863 9766258.4 766.53851 734661.5 766.53851 7566553.7 766.63357 721461.5 766.633357 721036.8 766
766.042838 72664709.7 766.076834 7660789.0 766.134971 61286850.0 766.171674 7325082.6 766.207409 7384172.0 766.224912 9312248.7 766.316365 7565533.6 766.338951 7506562.5 766.316308 7266717.1 766.40138 7286444.6 766.412633 8374147.2 766.422863 9766740.7 766.4242663 976740.7 766.4412633 8374147.2 766.442668 9766740.7 766.442648 7566258.4 766.51468 7566558.4 766.535818 7766018.4 766.535818 7766018.4 766.633367 8721036.8 766.63337 8721036.8 766.633367 8721036.8 766.78289 10044179.1 766.784883 24806535.7 766.78389 10044179.1 766.78289 102914179.1 766.78289 102941479.1 766.78289 102941479.1 766.782839 1044179.1
766.076334 7650789.0 766.113954 9107772.8 766.154971 61286850.0 766.154971 61286850.0 766.224912 9312248.7 766.36365 7565533.6 766.316365 7565533.6 766.41626 934242177.8 766.42633 7667617.1 766.42633 9766740.7 766.42633 9766740.7 766.42633 9766740.7 766.42633 9766740.7 766.42635 92467452.5 766.456620 7778964.5 766.456620 7778964.5 766.456620 7778964.5 766.514688 7566258.4 766.535018 7760018.4 766.53571 926426.5 766.633570 922190.5 766.663357 9229190.5 766.78108 10044179.1 766.782899 10044179.1 766.78108 10049591.5 766.78108 10045951.5 766.78108 10045951.5 766.78108 10045951.5 766.831702 1007457.4
766.113054 9107772.8 766.154971 61286850.0 766.207469 7384172.0 766.224912 9312248.7 766.316365 7565533.6 766.336365 7565533.6 766.417637 72509 766.420338 374147.2 766.4376809 32462177.8 766.441623 8374147.2 766.441624 6968114.6 766.442663 9766740.7 766.456620 7778964.5 766.456620 7778964.5 766.514688 7566258.4 766.535818 7766018.4 766.535818 7766018.4 766.63357 8721036.8 766.63357 8721036.8 766.63357 8721036.8 766.63357 8721036.8 766.73889 10044179.1 766.73889 10044179.1 766.73835 1204559.5 766.761708 10045591.5 766.78385 14580612.4 766.817063 10045591.5 766.817063 10045591.5 766.817063 10045591.8 <tr< td=""></tr<>
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768.071865	92901051.1	$C_{96}H_{123}N_{31}O_{50}P_9S_9$	768.071724	-	-4	c9 + 2H
				0.184		
768.103310	149855512.2					
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769.086864 769.101482	12211432.0 8131397.9	$C_{51}H_{66}N_{15}O_{25}P_4S_4$	769.102104	0.809	-2	z5 - B(dC) + 1H
769.124220 769.151848	7989118.8 29575117.8					
769.167239	21891305.7					
769.181344	9491329.4					
769.191818	8119120.9 8816240.0					
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769.234984	9280790.9					
769.264392	43875160.5					
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769.336137	7034019.1					
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769 770521	45588900 5					
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774 00007	05407000 4	11				IH
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				0.017		
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010.112303	0/943/2./		010 072010		Б	w12
019.073102	15540556.9	$C_{126}\Pi_{160}\Pi_{44}O_{66}\Gamma_{12}O$	019.073040	-	-0	WIZ
823 338965	15941860 2	12		0.104		
823 586277	12841415.6					
823 838104	11721384 7		823 839695	1 931	-4	a10
838 037967	17118344.9	0100113410330541 909	020.000000		•	
838 160431	13680471.0					
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858.245104	24569875.9					
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863.540613 863.622009 863.669581 863.690016 863.742958 863.794101 863.812968 863.873531 863.911102 863.930959 863.999201 864.044489 864.060318 864.190599 881.429354 881.763585	30456456.1 16230759.7 28428442.4 6954755.0 24896851.4 11049619.2 10541888.2 15805313.7 10999936.5 59169357.9 9157179.8 28743633.6 34526395.1 18432005.4 30731512.7 36108378.6	C ₈₆ H ₁₀₇ N ₂₆ O ₄₄ P ₇ S ₇	881.764150	0.641	-3	b8 - H2O, a8 -
882.095115 882.432794 887.097147	28213411.9 17508216.6 38087141.8	$C_{56}H_{73}N_{18}O_{29}P_5S_5$	887.096848	-	-2	w5
887.598473 888.095407 892.028580 897.281582 897.490715 901.928224 902.108499 902.273135 902.446854 903.041916 903.112826 908.531432 908.701856 908.869981 909.036925 909.341151 909.600032 909.847562 922.425899	20564042.2 15379331.4 7138695.0 9067102.2 8594083.1 12664794.7 9956741.9 13098591.9 9072733.1 6816826.7 17462435.3 1433223.3 17335175.0 13181447.1 10337608.1 11492177.5 10370016.7 13138697.4 32021112.2	C ₈₆ H ₁₁₀ N ₃₀ O ₄₄ P ₈ S ₈	922.424684	_	-3	w8
923.090975 923.427959 950.991004 958.041584 967.470197 967.613890 967.757693 967.900938 979.117683 984.191665 984.335479 984.481228 984.620918 984.906446 986.478745 986.621437 986.621437 986.765452 986.891349 986.908574 986.900502	24169173.5 14297625.2 6843093.9 9192465.5 9175102.6 12348946.2 10202367.7 8335023.4 7700500.8 12355787.1 15020440.6 15450198.8 9216482.2 8186525.1 7515548.8 30379061.6 50397702.1 14630271.3 37803636.5 7617235.7			1.317		

987.041067 987.057533 987.133593 987.181471 987.208915 987.333111 987.350783 987.644083 987.767679 987.919835 989.604414 989.849791 989.902275	25038811.2 23155637.9 9249860.6 9553756.6 14909817.2 15988680.1 17650542.9 20778677.0 27360600.0 9001970.1 7918685.6 11652214.7 16627351.2					
990.045534 990.101709	6784933.6 9883677.7	$\begin{array}{c} C_{31}H_{34}N_{10}O_{16}P_3S_3\\ C_{126}H_{159}N_{40}O_{65}P_{11}S\\ {}^{11}\end{array}$	990.045648 990.102912	0.115 1.215	-1 -4	x3 - B(dC) - 4H a12
990.332223 1024.09369 5	15735595.8 17325694.8	$C_{126}H_{160}N_{44}O_{66}P_{12}S_{12}$	1024.09313 0	- 0.552	-4	w12
1024.59386 5	23680214.9					
1024.84373	15654884.1					
1037.42946	8761831.7					
1037.76563	10246394.0					
1038.10063	8877070.9	$C_{131}H_{166}N_{41}O_{68}P_{12}S$	1038.10001	-	-4	a13 - B(T)
8 1052.10039 3	20312183.6	${\overset{_{12}}{C_{65}}}{H_{82}}{N_{23}}{O_{34}}{P_6}{S_6}$	9 1052.09994 9	0.596 - 0.422	-2	w6 - CH3
1052.50199	65765968.9		•	•••==		
1052.70190	57797811.6					
, 1052.90316	41694668.8					
1053.10448	21134328.6					
o 1053.30344	15914960.1					
3 1055.70117	21847097.9					
3 1055.90133	20703807.7					
0 1057.70147	8922578.9					
0 1057.90046	9687990.8					
6 1059.61078	8378460.2	$C_{66}H_{85}N_{23}O_{34}P_6S_6$	1059.61168 6	0.855	-2	w6
1075.61062	18157275.7	$C_{136}H_{170}N_{46}O_{69}P_{12}S$	1075.61041	-	-4	z13 - 2H, y13 - H2O
1075.86059	21566338.9	12	5	0.190		
0 1076.10952	31789891.9					
1076.36249	19918459.5					
4 1076.60974	11074148.9					

4 1077.11505	9716309.0					
1079.72018	9631687.1					
3 1080.11064	8700829.1	$C_{136}H_{172}N_{46}O_{70}P_{12}S_{12}$	1080.11305 6	2.235	-4	y13
2 1082.21699 2	8519980.8					
2 1082.31042 7	91427515.1	C ₁₇₂ H ₂₁₅ N ₅₆ O ₈₈ P ₁₅ S	1082.31162 6	1.108	-5	M - 7H
1082.42000 0	17807981.2					
0 1082.61934 7	27936228.5					
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1083.11329 7	217877851.8					
1083.20654	10912824.6					
1083.30255 3	24410733.2					
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0 1151.63887 1	8612569.8					
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1382.68691	18903335.0					
1			Abs mean error	0.788		
			Abs mean	0.677		

std dev

Supporting References

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