

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051722\
 Data File : BG053588.D
 Acq On : 17 May 2022 17:46
 Operator : CG/JU
 Sample : N2870-11
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RB-220511

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.167	297	303	311	rBV	73106	116332	4.14%	1.042%
2	5.649	379	385	397	rBV	284033	489529	17.44%	4.383%
3	7.246	649	657	674	rBV	190123	357429	12.74%	3.200%
4	8.081	792	799	806	rBV	117279	202450	7.21%	1.813%
5	9.244	989	997	1014	rVB	423906	770539	27.45%	6.899%
6	10.894	1270	1278	1287	rBV	152750	289216	10.30%	2.590%
7	12.187	1490	1498	1509	rBV4	13737	32409	1.15%	0.290%
8	13.332	1684	1693	1706	rBV	1144637	1800735	64.16%	16.123%
9	14.707	1919	1927	1936	rVB	285746	446426	15.91%	3.997%
10	16.199	2174	2181	2197	rBV	907735	1465194	52.20%	13.119%
11	17.450	2388	2394	2402	rBV	365606	558118	19.89%	4.997%
12	18.108	2501	2506	2511	rBV2	56426	68786	2.45%	0.616%
13	20.059	2832	2838	2844	rBV	2167425	2806651	100.00%	25.130%
14	21.733	3117	3123	3130	rVB2	309273	516311	18.40%	4.623%
15	23.207	3366	3374	3393	rBV	354514	735180	26.19%	6.583%
16	25.017	3671	3682	3697	rVB2	166929	513160	18.28%	4.595%

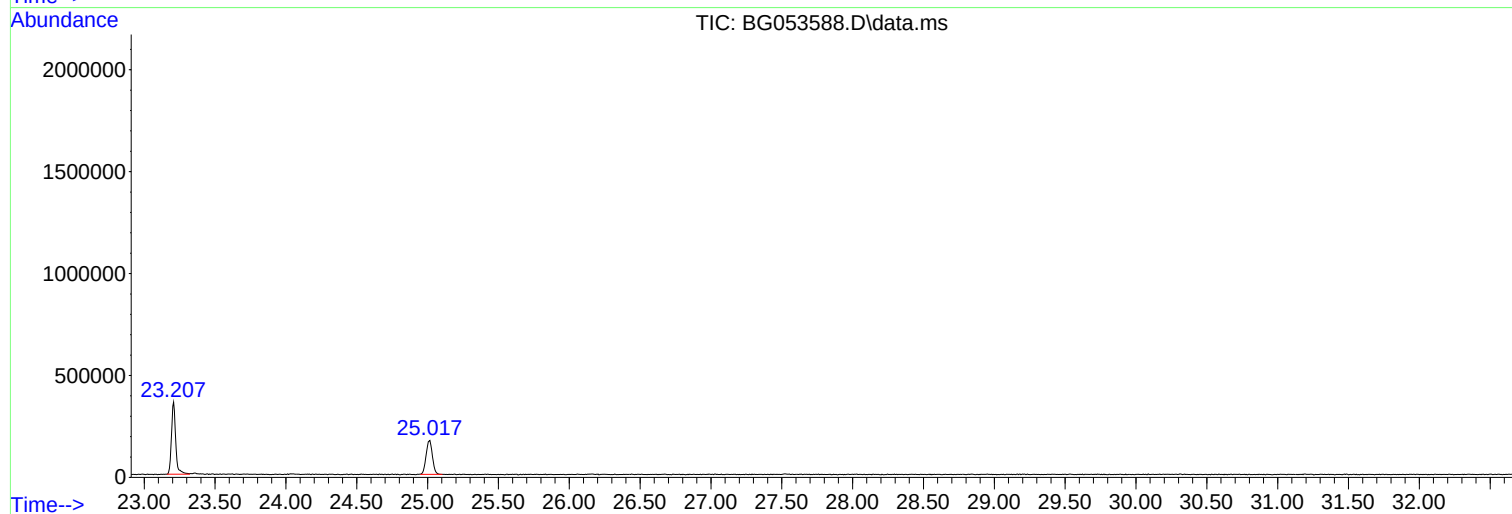
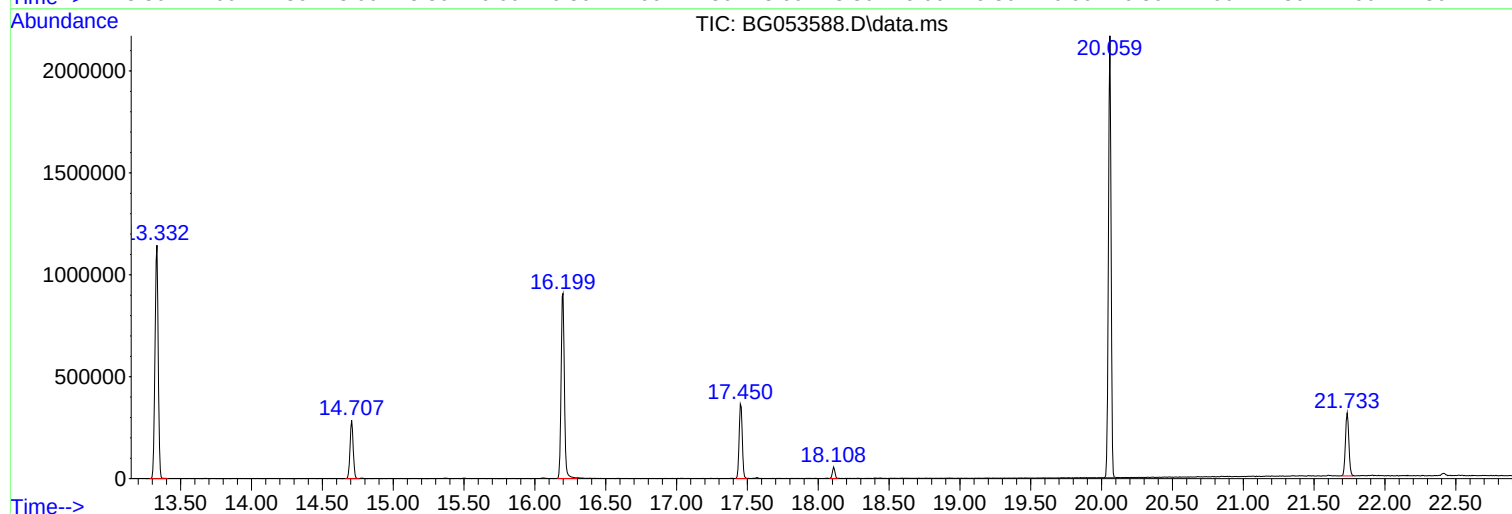
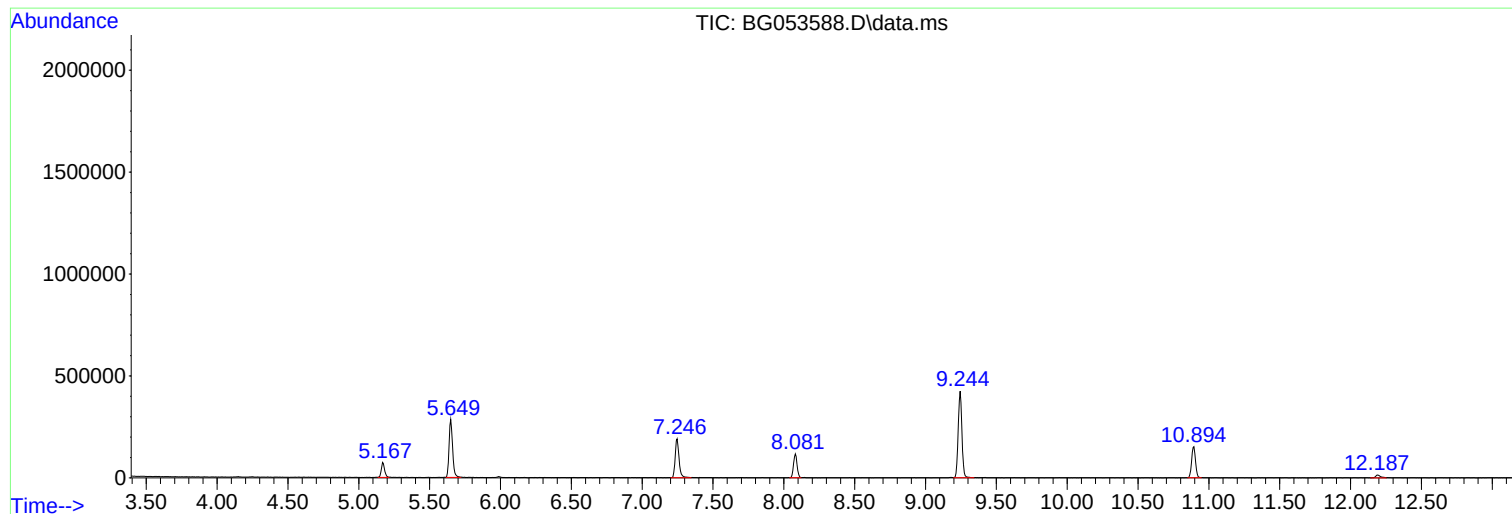
Sum of corrected areas: 11168465

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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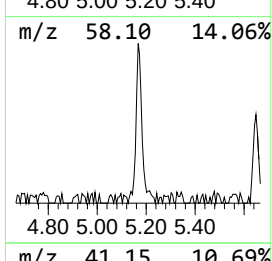
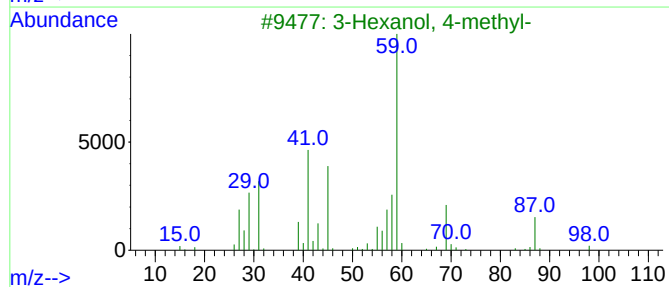
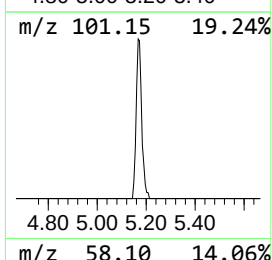
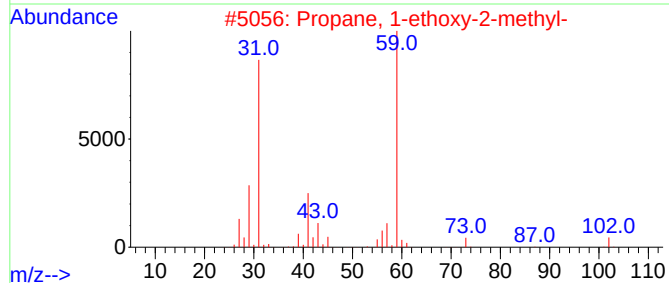
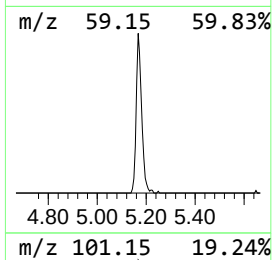
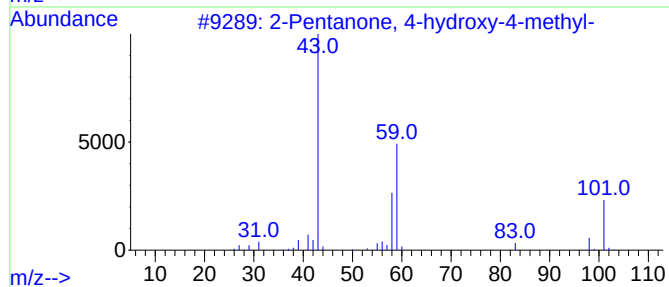
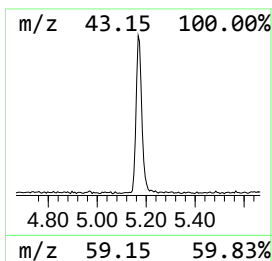
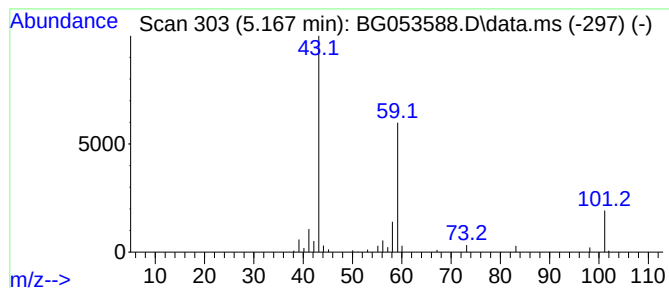
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.167	11.49 ng	116332	1,4-Dichlorobenzene-d4	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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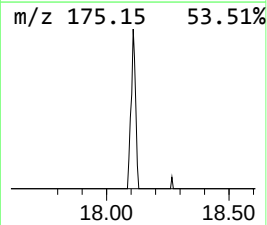
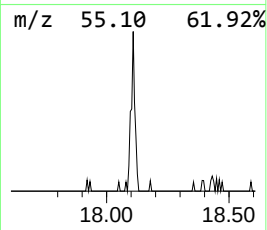
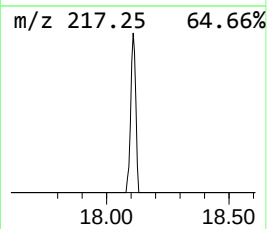
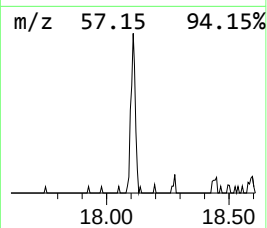
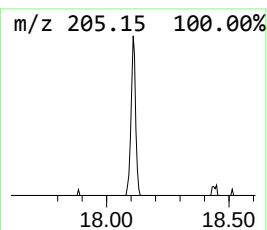
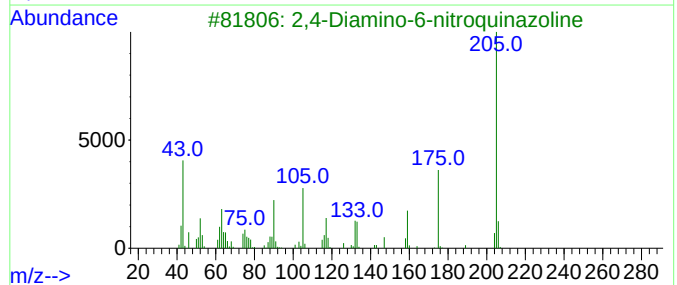
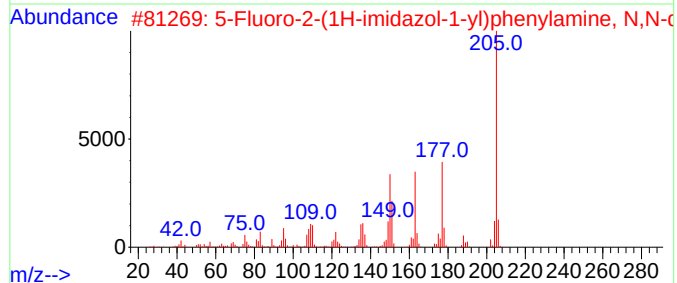
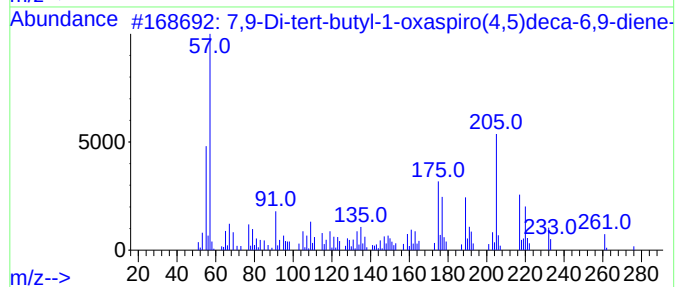
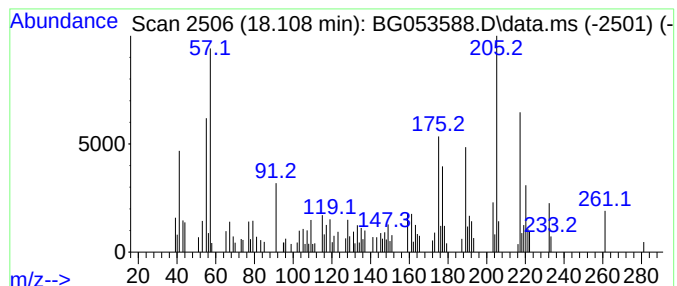
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Peak Number 2 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.108	2.46 ng	68786	Phenanthrene-d10	17.450

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	83		
2	5-Fluoro-2-(1H-imidazol-1-yl)phe...	205	C11H12FN3	1000512-19-0	38		
3	2,4-Diamino-6-nitroquinazoline	205	C8H7N5O2	007154-34-9	38		
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38		
5	Benzenamine, N,N-diethyl-4-(2-ni...	220	C12H16N2O2	064462-51-7	38		



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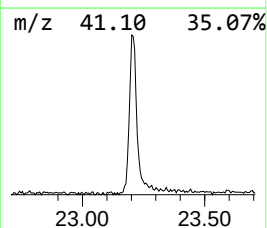
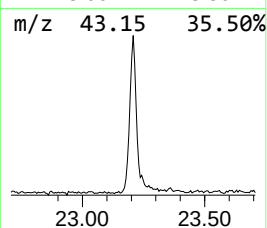
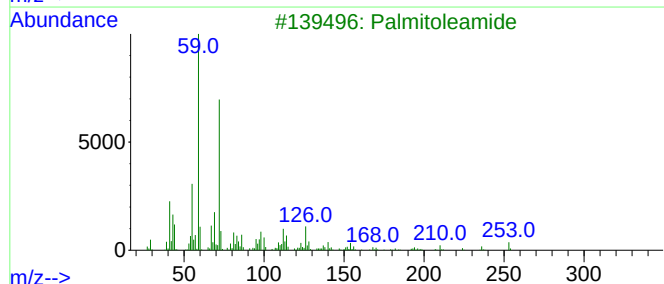
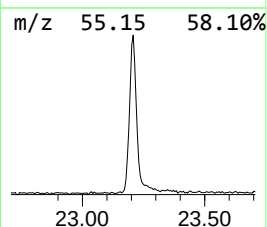
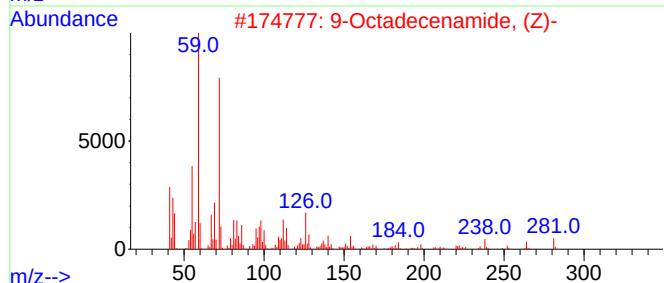
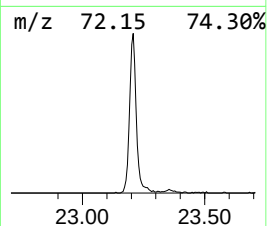
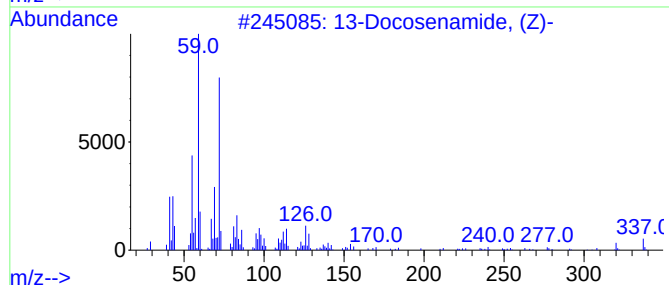
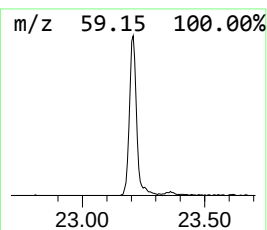
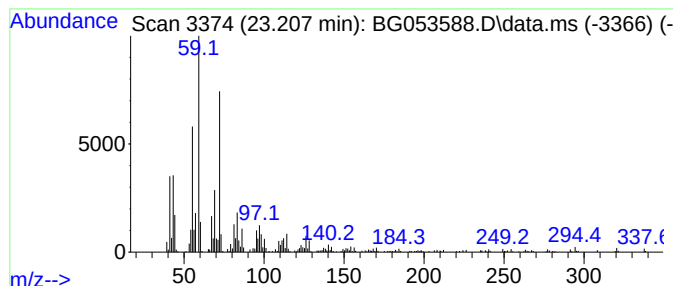
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Peak Number 3 13-Docosenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.207	28.48 ng	735180	Chrysene-d12	21.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	98
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
3			Palmitoleamide	253	C16H31NO	106010-22-4	72
4			Dodecanamide	199	C12H25NO	001120-16-7	43
5			Tetradecanamide	227	C14H29NO	000638-58-4	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.167	11.5	ng	116332	1	8.081	202450	20.0
7,9-Di-tert-but...	18.108	2.5	ng	68786	4	17.450	558118	20.0
13-Docosenamide...	23.207	28.5	ng	735180	5	21.733	516311	20.0