

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059742.D
 Acq On : 17 Nov 2023 22:57
 Operator : MA/JU
 Sample : 05311-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-3

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.834	408	416	426	rBV	329913	538026	26.20%	6.084%
2	7.455	686	692	701	rVB	400898	682606	33.24%	7.719%
3	8.337	837	842	850	rVB2	108850	187265	9.12%	2.118%
4	9.541	1039	1047	1054	rVB	249770	451333	21.98%	5.104%
5	11.186	1321	1327	1336	rBV	150102	280491	13.66%	3.172%
6	13.589	1729	1736	1743	rBV	768152	1163705	56.67%	13.160%
7	14.970	1964	1971	1977	rVB2	245851	407632	19.85%	4.610%
8	16.451	2216	2223	2232	rBV2	736420	1074089	52.31%	12.146%
9	17.720	2432	2439	2444	rBV	356053	552130	26.89%	6.244%
10	17.814	2450	2455	2461	rVB6	15315	23518	1.15%	0.266%
11	18.531	2571	2577	2586	rBV3	133223	191222	9.31%	2.162%
12	19.664	2764	2770	2776	rBV8	10774	32694	1.59%	0.370%
13	19.788	2787	2791	2797	rVB3	57143	66089	3.22%	0.747%
14	20.293	2871	2877	2883	rBV	1652457	2053334	100.00%	23.220%
15	21.580	3092	3096	3102	rBV4	58497	86614	4.22%	0.979%
16	22.044	3168	3175	3181	rBV	289921	519611	25.31%	5.876%
17	25.622	3774	3784	3797	rVB2	166371	532624	25.94%	6.023%

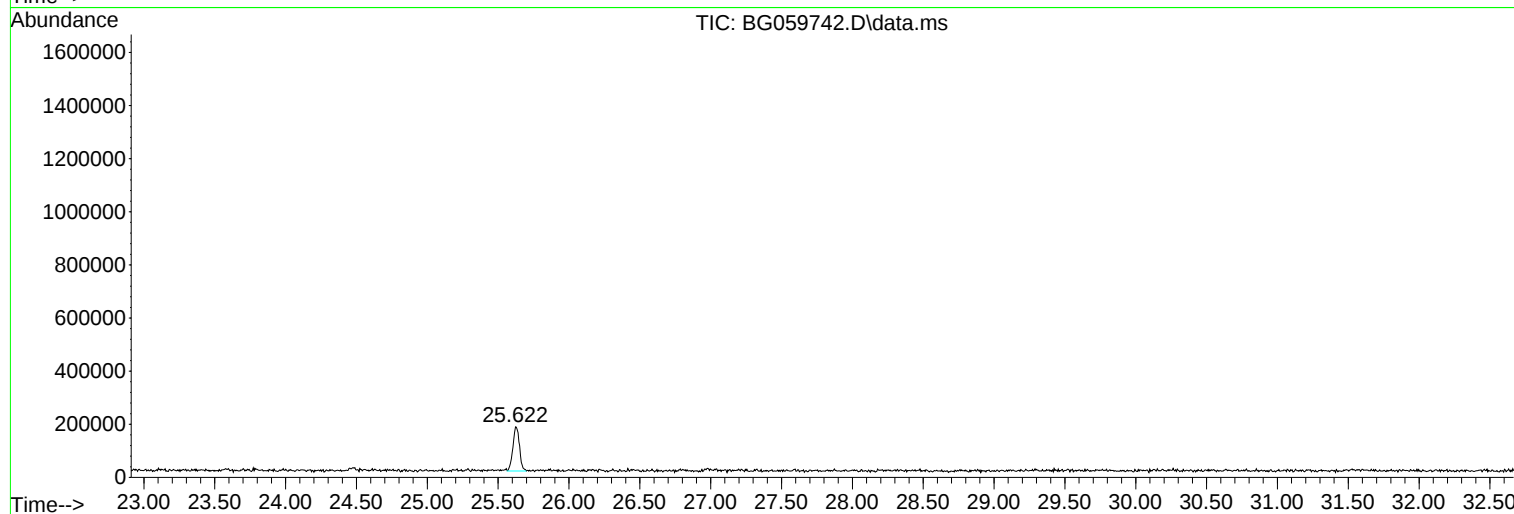
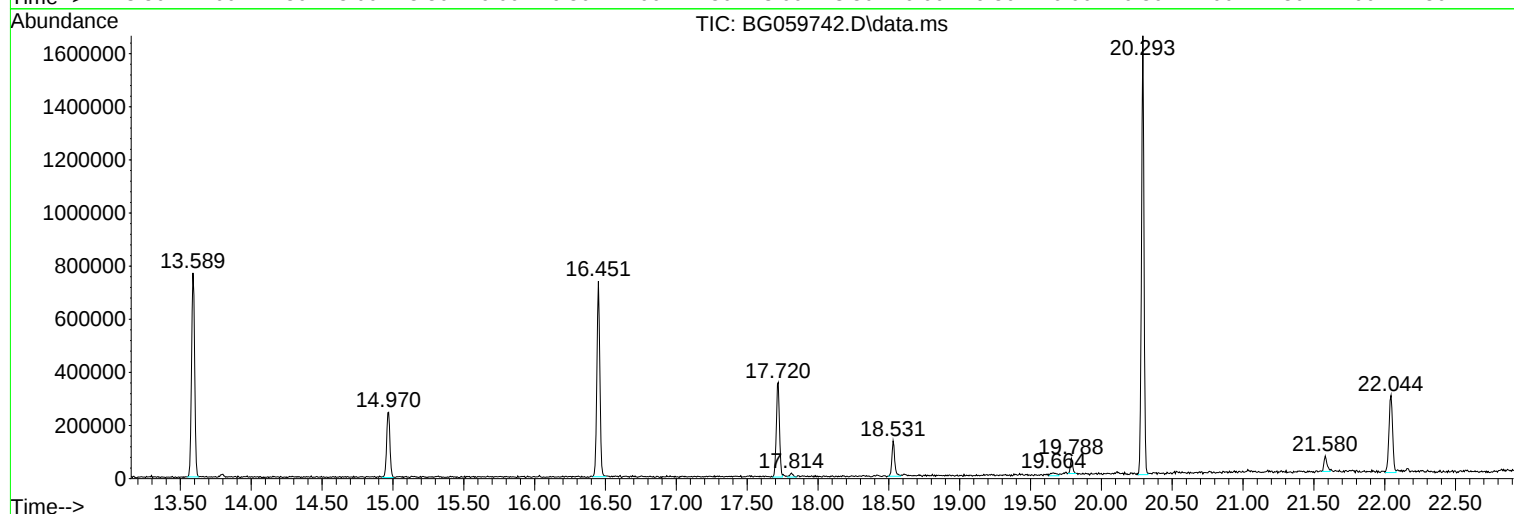
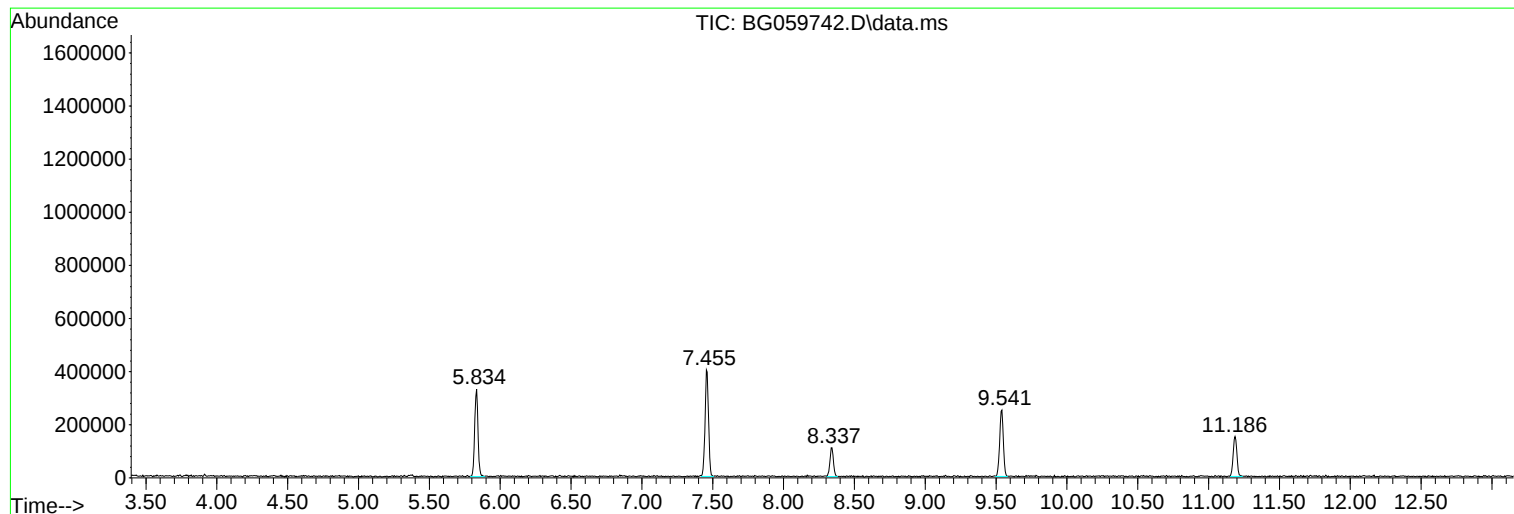
Sum of corrected areas: 8842983

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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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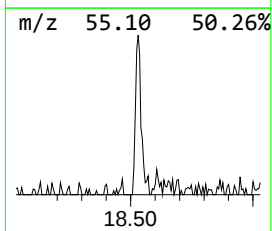
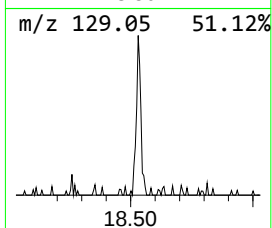
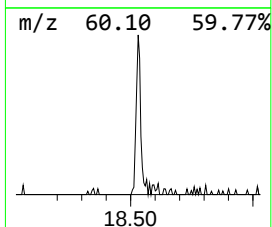
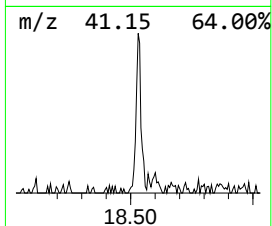
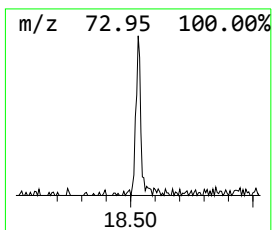
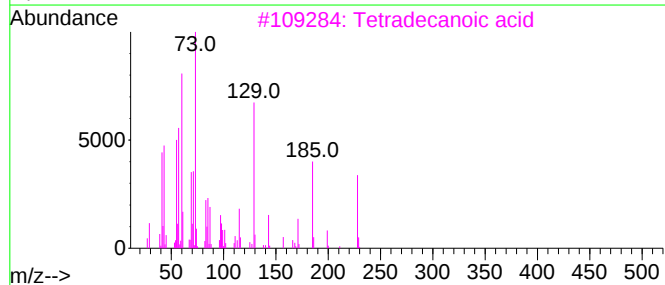
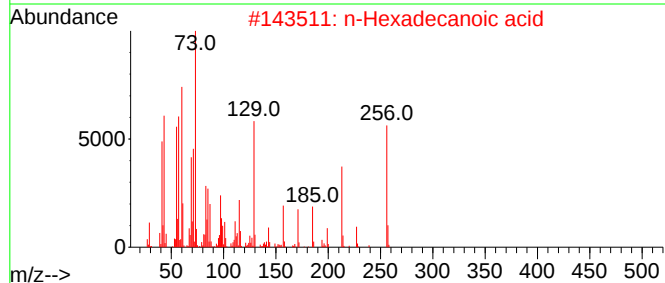
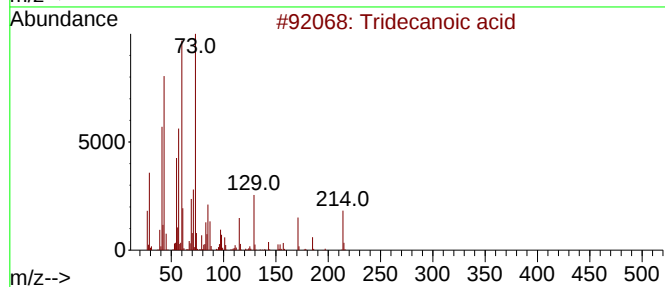
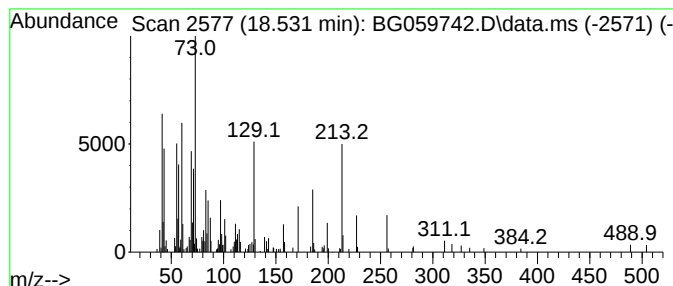
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.531	6.93 ng	191222	Phenanthrene-d10		17.720	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tridecanoic acid		214	C13H26O2	000638-53-9	83
2	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	70
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	58
4	n-Decanoic acid		172	C10H20O2	000334-48-5	27
5	Undecanoic acid		186	C11H22O2	000112-37-8	27



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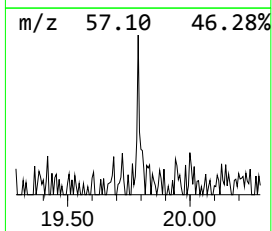
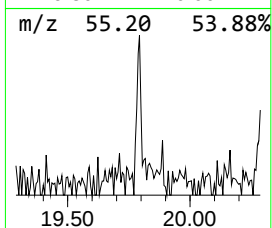
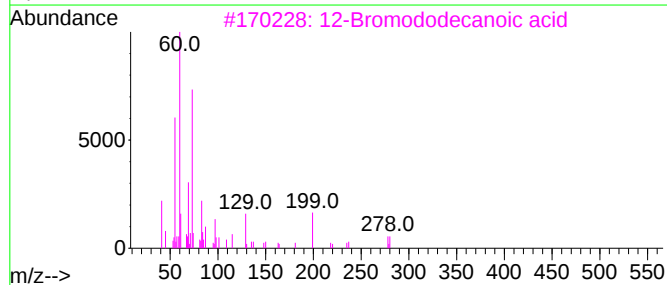
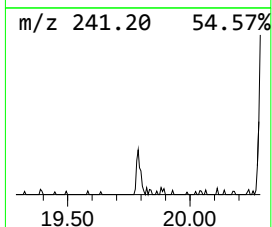
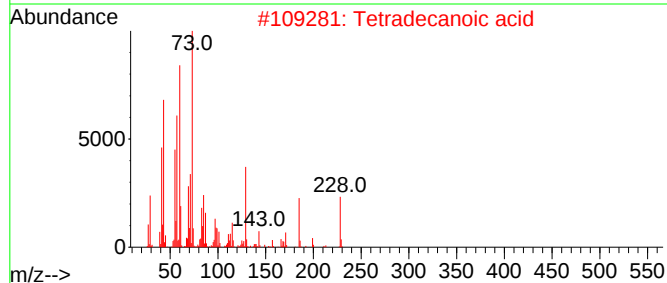
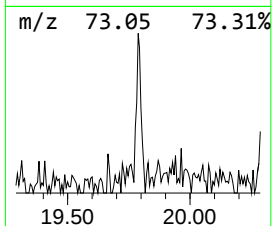
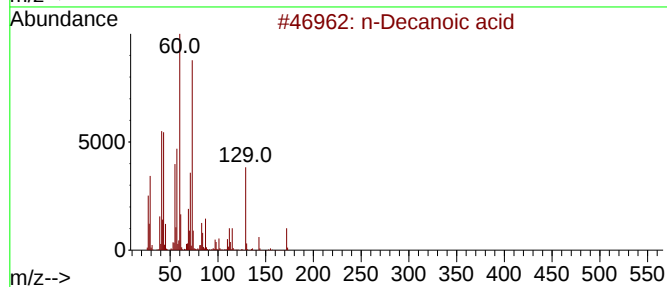
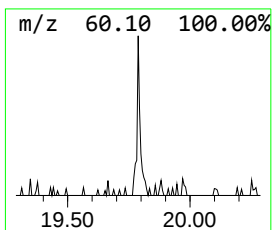
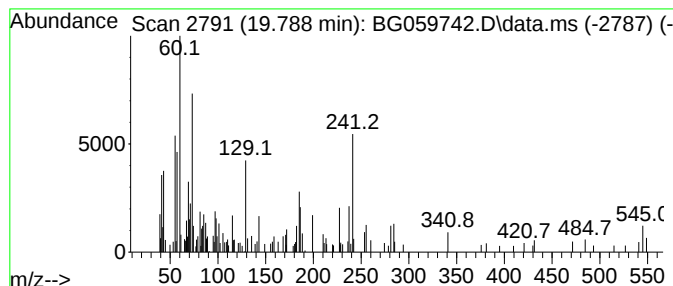
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Peak Number 2 unknown19.788 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.788	2.39 ng	66089	Phenanthrene-d10	17.720

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	43
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	43
3		12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	38
4		1,6-Anhydro-.beta.-d-talopyranose	162	C6H10O5	1000133-05-8	22
5		Octadecanoic acid	284	C18H36O2	000057-11-4	18



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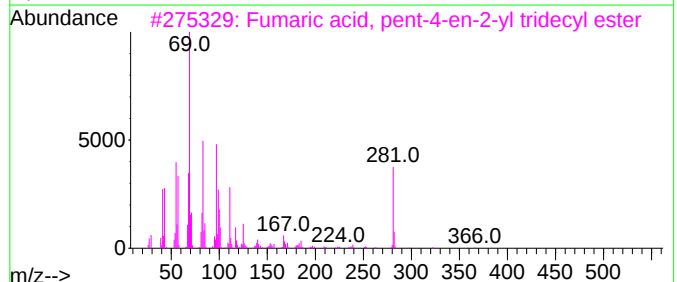
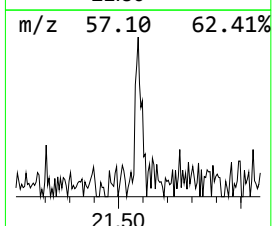
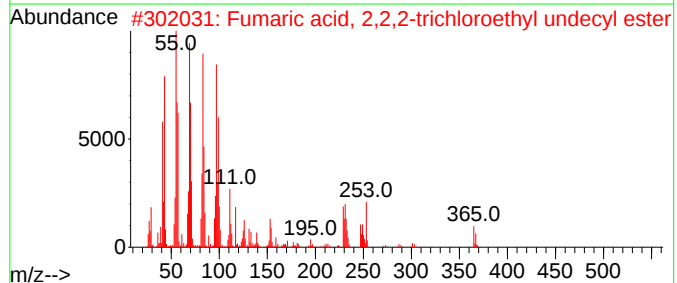
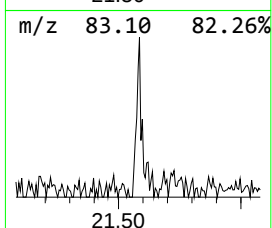
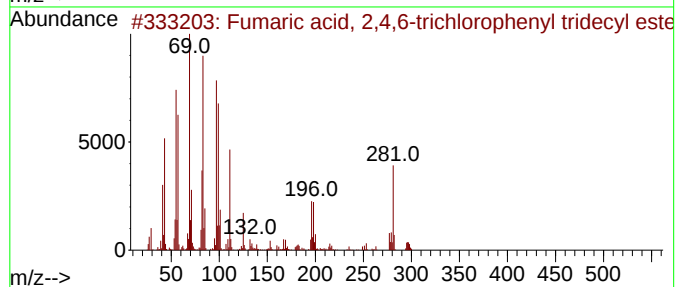
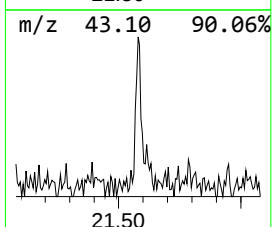
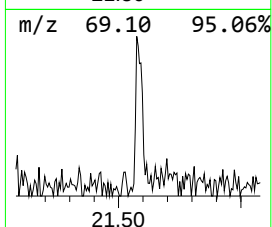
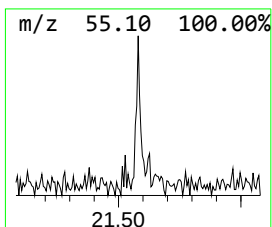
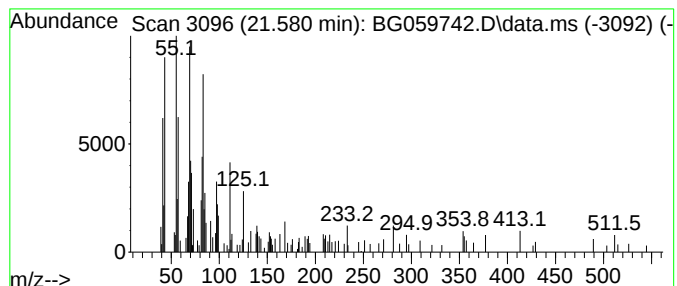
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Peak Number 3 unknown21.580 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.580	3.33 ng	86614	Chrysene-d12	22.044

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, 2,4,6-trichlorophe...	476	C23H31Cl3O4	1000348-27-7	40
2			Fumaric acid, 2,2,2-trichloroeth...	400	C17H27Cl3O4	1000348-50-8	36
3			Fumaric acid, pent-4-en-2-yl tri...	366	C22H38O4	1000348-93-2	23
4			Fumaric acid, 2,4-dimethylpent-3...	480	C30H56O4	1010348-56-0	23
5			Cyclopentanecarboxamide, N-octad...	365	C24H47NO	1000419-71-7	22



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tridecanoic acid	18.531	6.9	ng	191222	4	17.720	552130	20.0
unknown19.788	19.788	2.4	ng	66089	4	17.720	552130	20.0
unknown21.580	21.580	3.3	ng	86614	5	22.044	519611	20.0