

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG041723\
 Data File : BG057122.D
 Acq On : 17 Apr 2023 22:35
 Operator : CG/JU
 Sample : 02366-08
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20230339-COMP-17

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-BG033023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.426	315	321	330	rBB	84565	129036	10.60%	2.162%
2	5.908	397	403	411	rBV	301417	495436	40.69%	8.302%
3	7.535	671	680	690	rBV	419960	727758	59.76%	12.195%
4	8.398	821	827	833	rBB	61530	100412	8.25%	1.683%
5	9.573	1020	1027	1038	rBB	225382	409231	33.61%	6.857%
6	11.236	1302	1310	1317	rBV	84141	147921	12.15%	2.479%
7	13.638	1712	1719	1727	rVB	573832	847027	69.56%	14.193%
8	15.013	1946	1953	1959	rVB	139276	216672	17.79%	3.631%
9	16.493	2199	2205	2215	rBV	464987	690774	56.73%	11.575%
10	17.750	2412	2419	2424	rBV	180470	268904	22.08%	4.506%
11	18.585	2556	2561	2571	rBV3	36366	60323	4.95%	1.011%
12	19.777	2761	2764	2770	rBV	12961	17315	1.42%	0.290%
13	19.842	2771	2775	2781	rVB4	8037	12317	1.01%	0.206%
14	20.135	2822	2825	2832	rVB	12045	17998	1.48%	0.302%
15	20.318	2851	2856	2862	rVB	967814	1217730	100.00%	20.405%
16	21.628	3073	3079	3085	rBV3	37644	67961	5.58%	1.139%
17	22.068	3145	3154	3160	rBV	150278	280442	23.03%	4.699%
18	25.605	3743	3756	3765	rBV	85964	260619	21.40%	4.367%

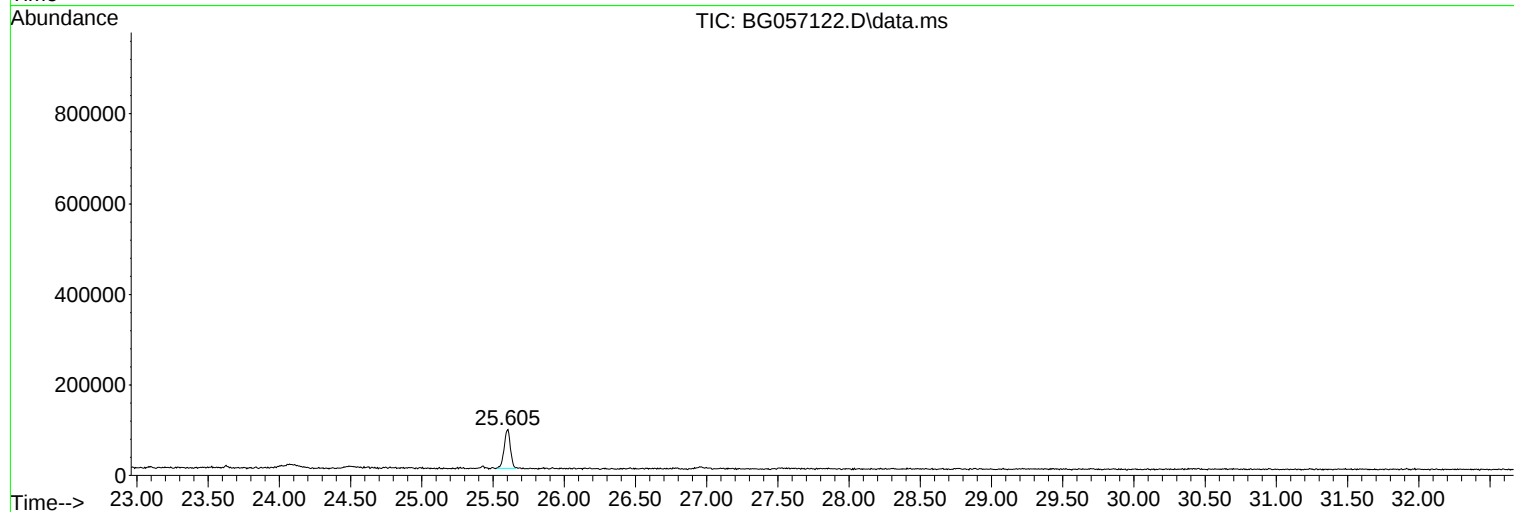
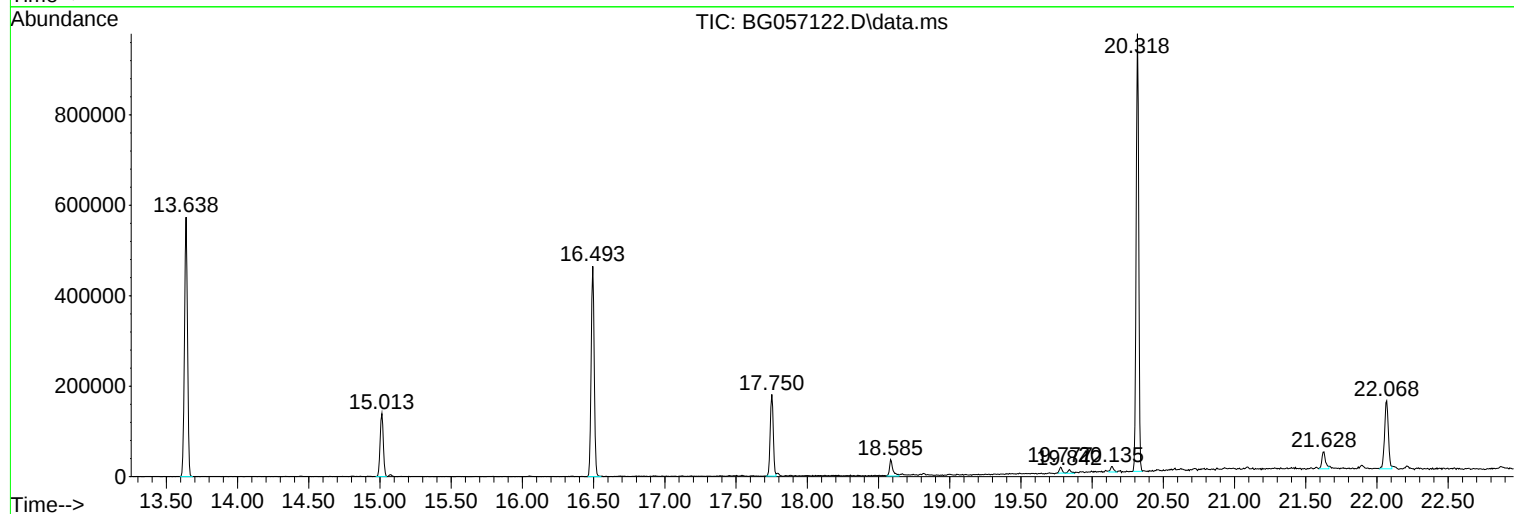
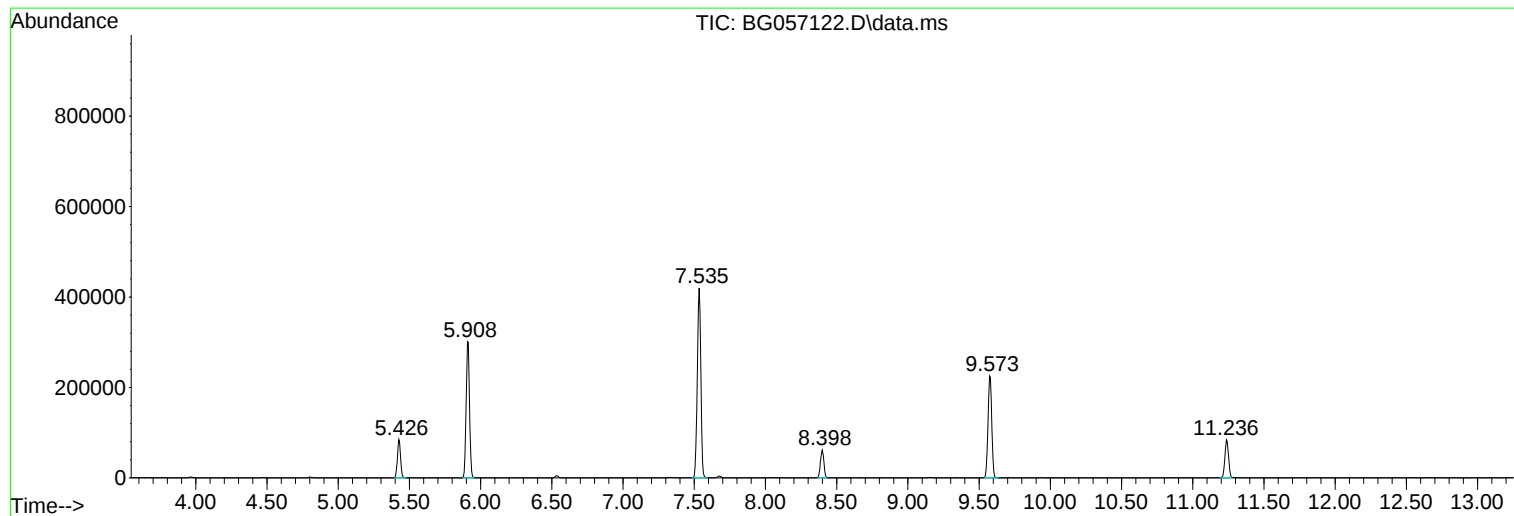
Sum of corrected areas: 5967876

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.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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20230339-COMP-17

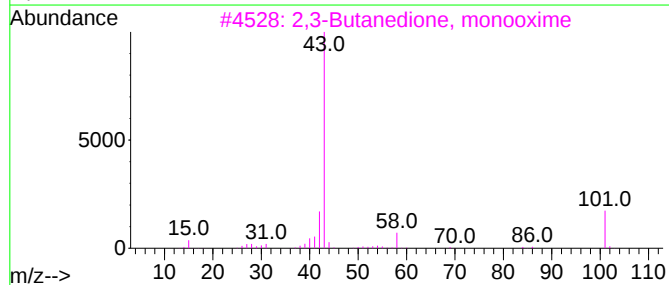
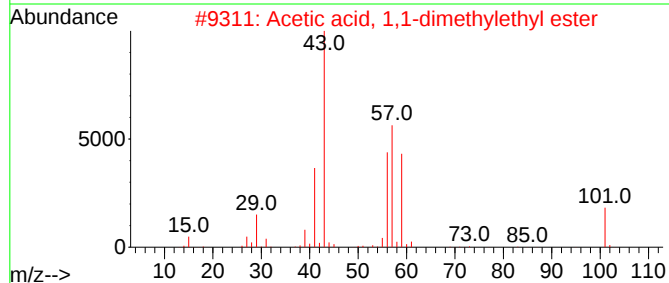
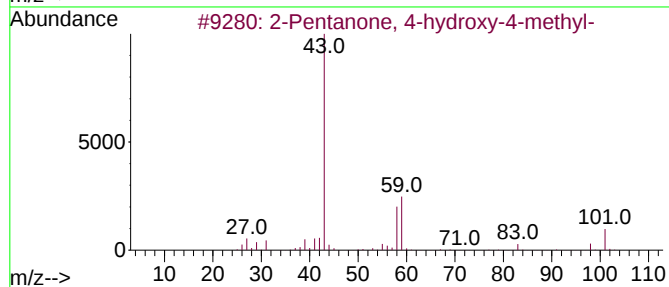
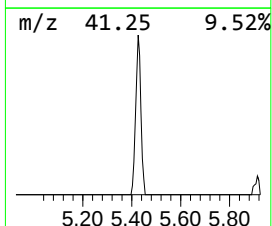
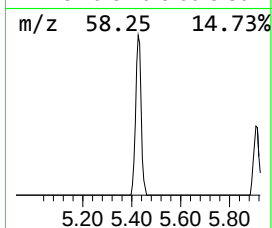
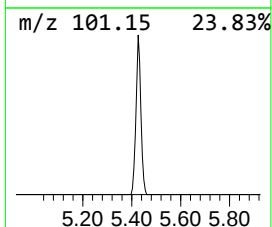
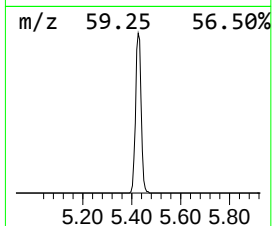
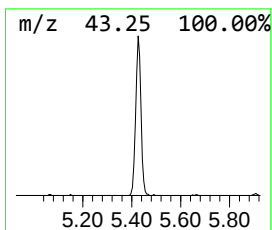
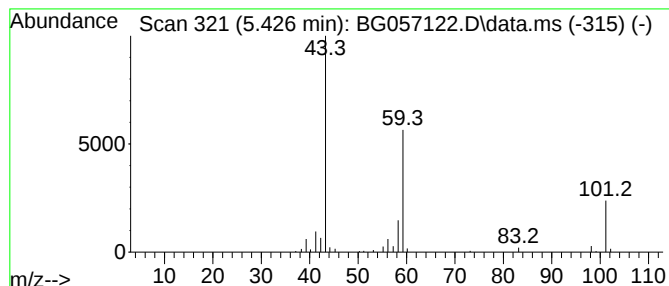
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.426	25.70 ng	129036	1,4-Dichlorobenzene-d4	8.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Propanenitrile, 3-ethoxy-	99	C5H9NO	002141-62-0	9		



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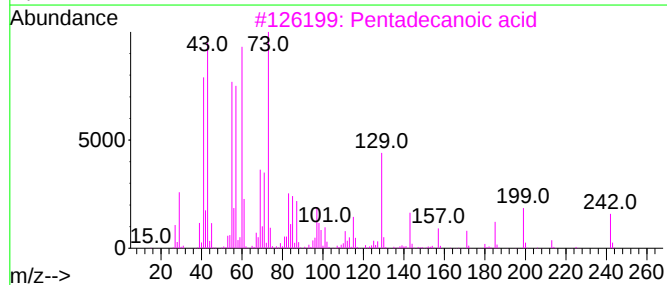
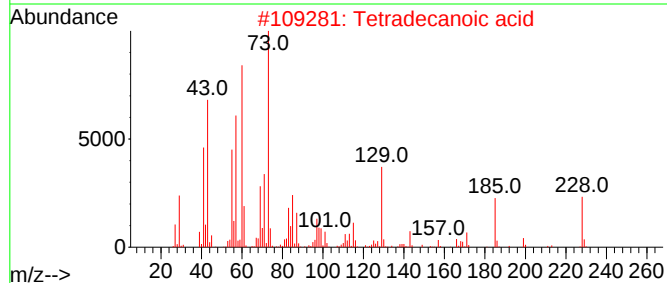
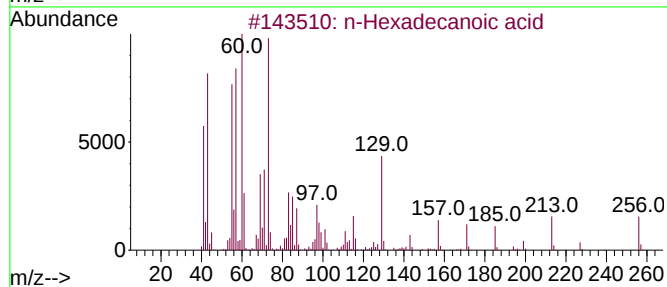
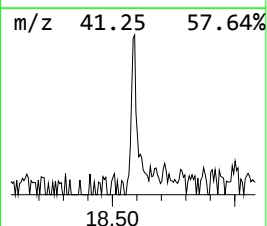
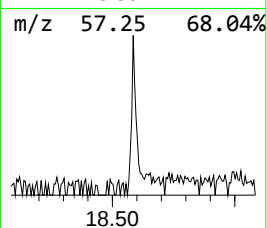
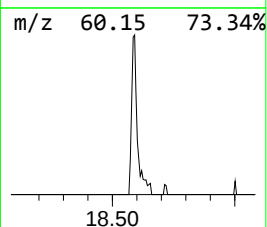
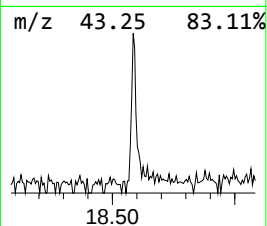
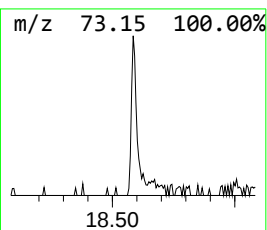
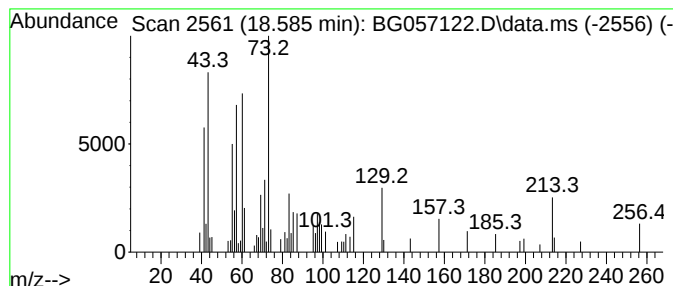
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG033023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.585	4.49 ng	60323	Phenanthrene-d10	17.750

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	62
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4			Tridecanoic acid	214	C13H26O2	000638-53-9	60
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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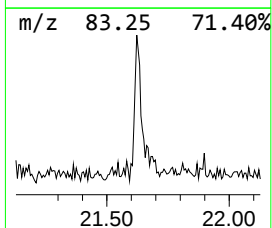
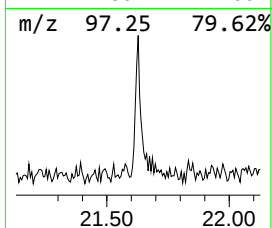
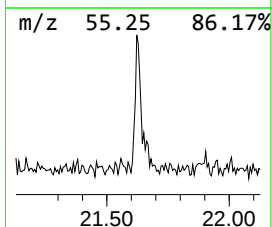
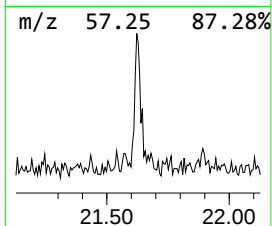
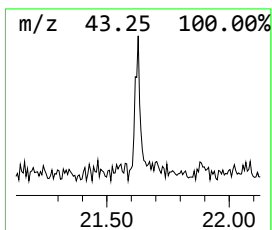
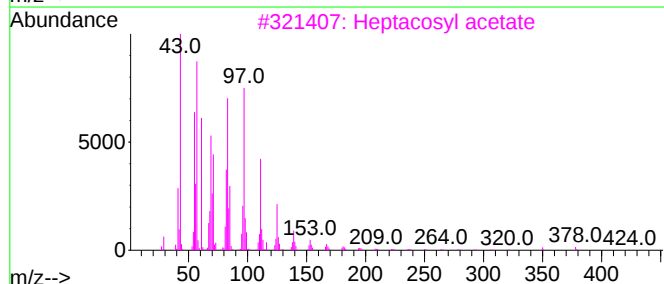
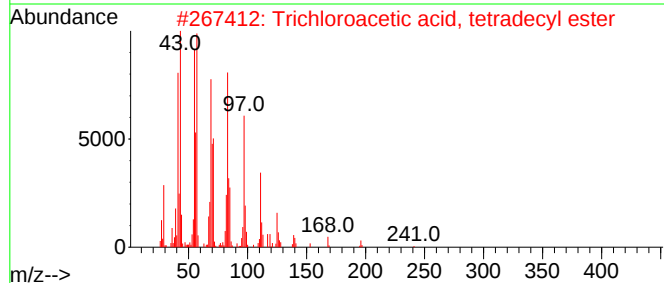
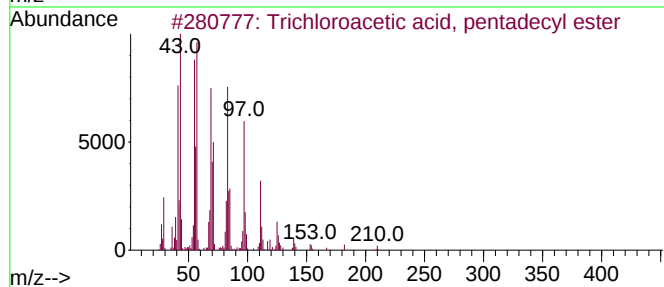
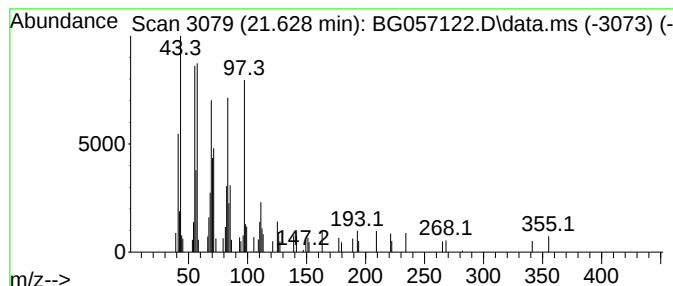
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Trichloroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.628	4.85 ng	67961	Chrysene-d12	22.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
2			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	76
3			Heptacosyl acetate	438	C29H58O2	1000351-78-2	74
4			9-Eicosene, (E)-	280	C20H40	074685-29-3	70
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.426	25.7	ng	129036	1	8.398	100412	20.0
n-Hexadecanoic ...	18.585	4.5	ng	60323	4	17.750	268904	20.0
Trichloroacetic...	21.628	4.8	ng	67961	5	22.068	280442	20.0