

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
 Data File : BG047972.D
 Acq On : 22 Jan 2021 3:29
 Operator : CG/JU
 Sample : M1153-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FK-PS-01-068

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-BG012121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG047972.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.702	395	402	411	rBV	758383	1165479	46.20%	7.244%
2	7.294	664	673	684	rVB	739471	1363486	54.05%	8.475%
3	8.146	810	818	824	rBV	191698	321415	12.74%	1.998%
4	9.309	1006	1016	1024	rBV	463329	831622	32.97%	5.169%
5	10.960	1289	1297	1304	rBV	247467	442510	17.54%	2.750%
6	13.393	1704	1711	1719	rVB	1176750	1797387	71.25%	11.171%
7	14.210	1844	1850	1855	rBV	67236	97711	3.87%	0.607%
8	14.768	1939	1945	1954	rVB2	423170	652626	25.87%	4.056%
9	16.248	2190	2197	2207	rBV	1014807	1571962	62.31%	9.770%
10	17.512	2405	2412	2419	rBV	527507	794443	31.49%	4.938%
11	18.393	2557	2562	2573	rBV	237775	334052	13.24%	2.076%
12	19.550	2755	2759	2765	rVB5	19231	38498	1.53%	0.239%
13	19.656	2774	2777	2786	rBV2	81281	118867	4.71%	0.739%
14	20.114	2849	2855	2861	rVB	1951422	2522728	100.00%	15.680%
15	21.431	3074	3079	3088	rVB2	280894	421358	16.70%	2.619%
16	21.795	3134	3141	3147	rBV	540284	912184	36.16%	5.670%
17	22.641	3279	3285	3292	rVB4	124725	275398	10.92%	1.712%
18	24.192	3542	3549	3557	rBV2	259832	575801	22.82%	3.579%
19	25.103	3694	3704	3713	rBV2	307452	885165	35.09%	5.502%
20	26.366	3912	3919	3931	rVB2	120826	364428	14.45%	2.265%
21	26.483	3933	3939	3951	rVB5	76387	249742	9.90%	1.552%
22	30.643	4634	4647	4648	rBV9	140566	352253	13.96%	2.189%

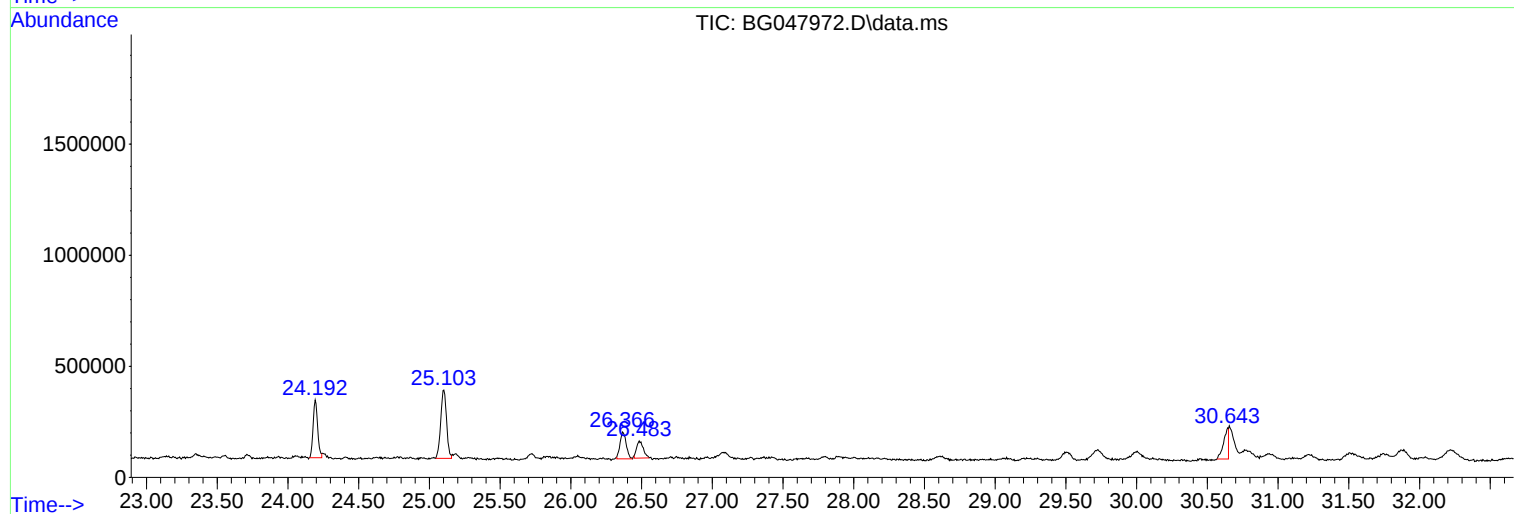
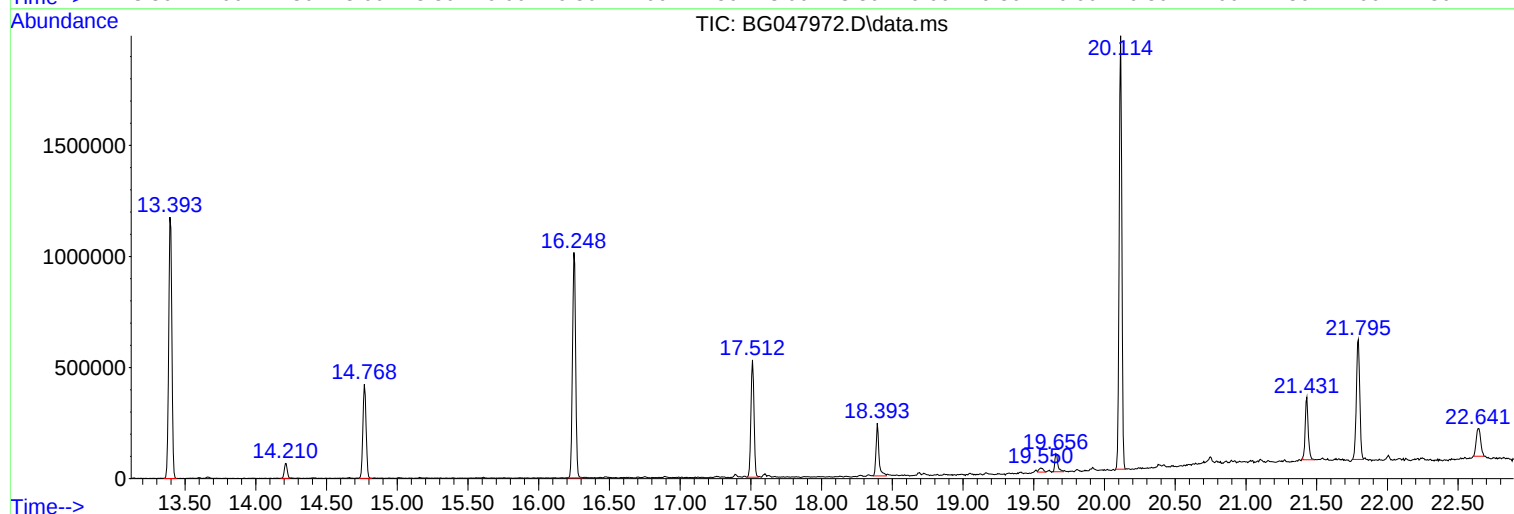
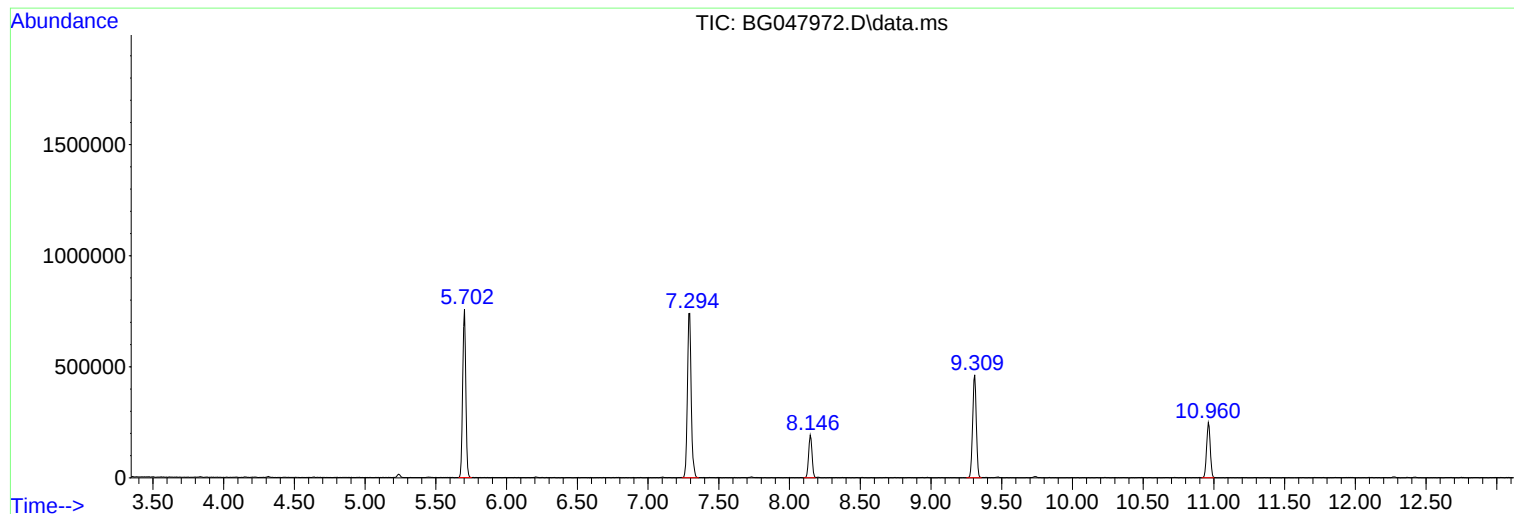
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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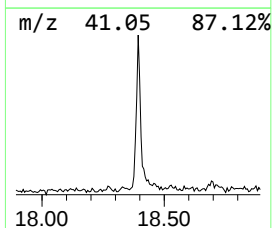
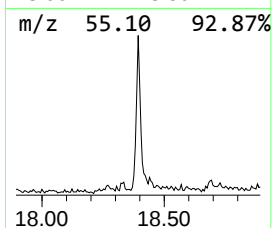
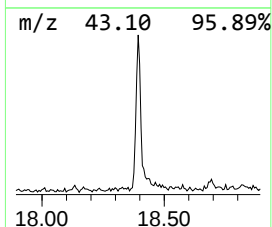
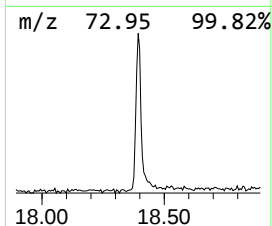
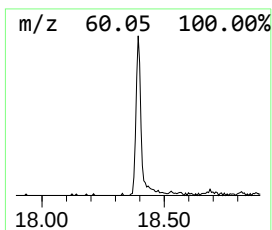
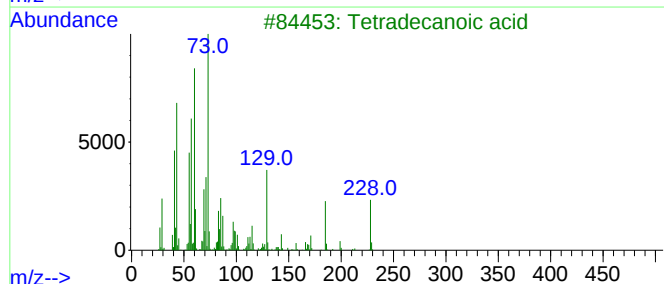
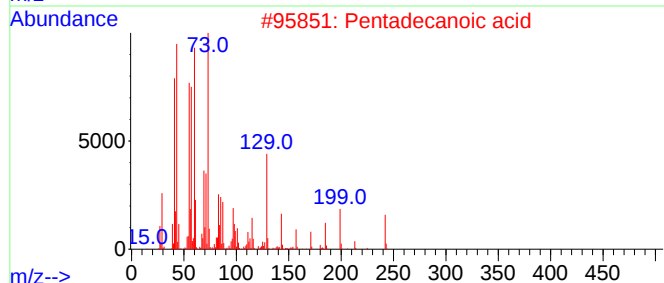
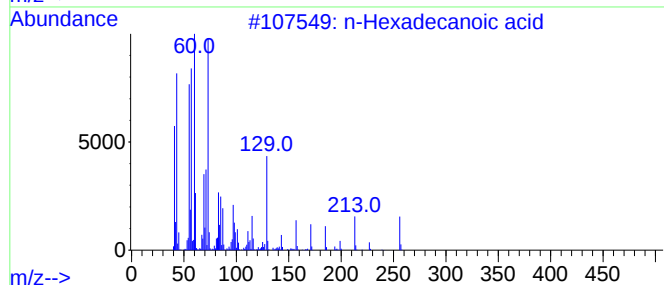
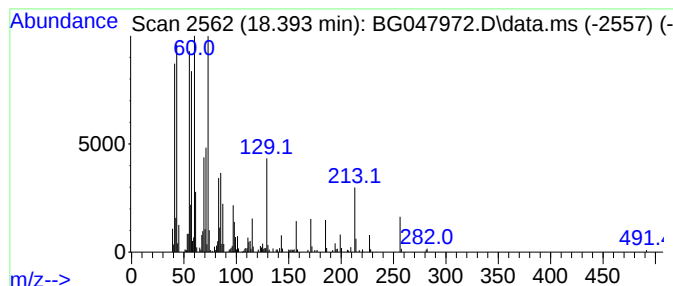
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.393	8.41 ng	334052	Phenanthrene-d10	17.512

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



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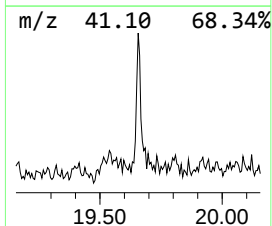
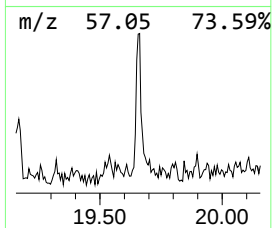
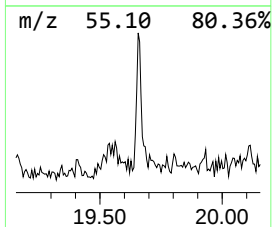
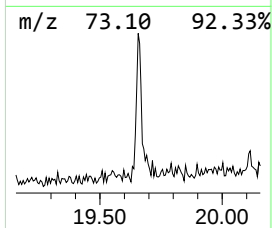
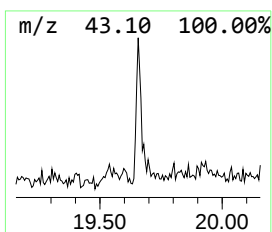
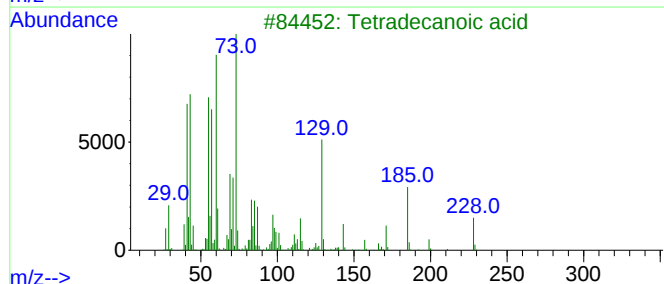
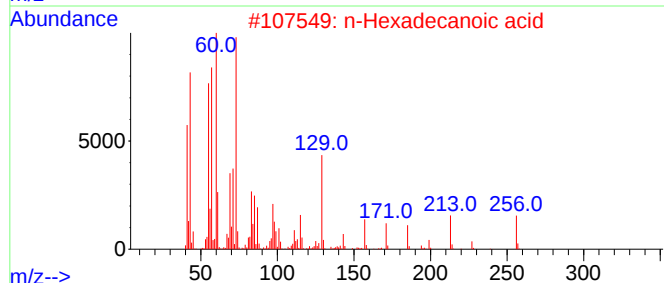
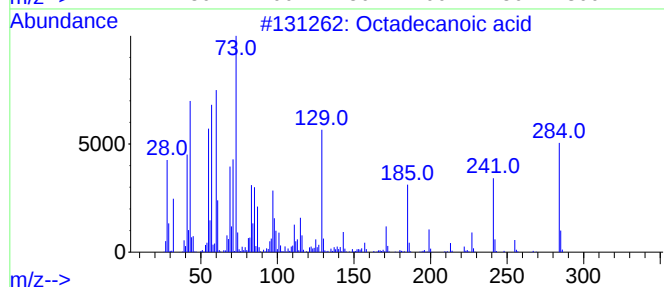
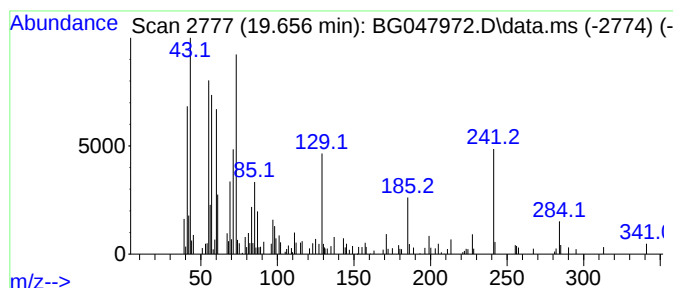
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 2 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.656	2.61 ng	118867	Chrysene-d12	21.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	87
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5			Tridecanoic acid	214	C13H26O2	000638-53-9	43



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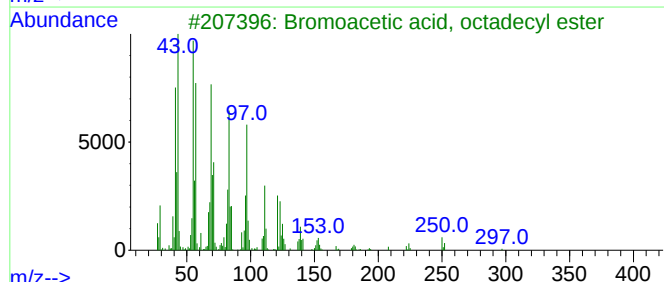
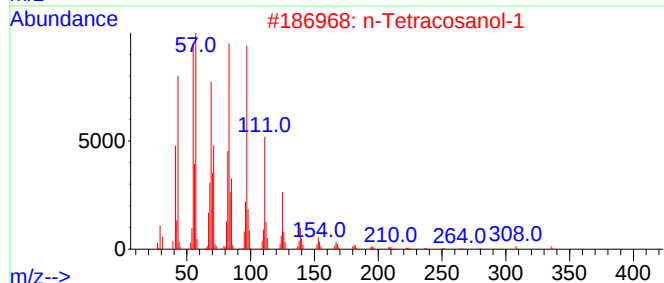
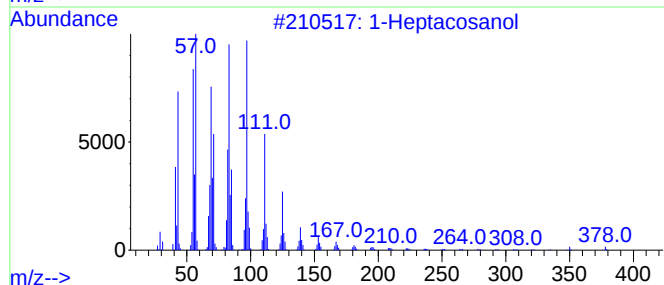
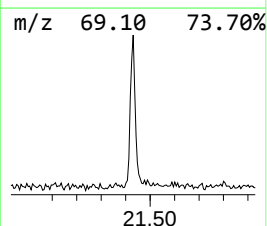
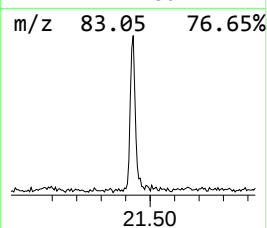
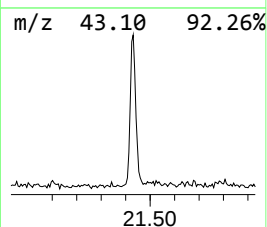
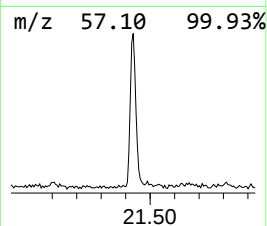
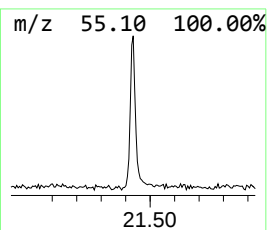
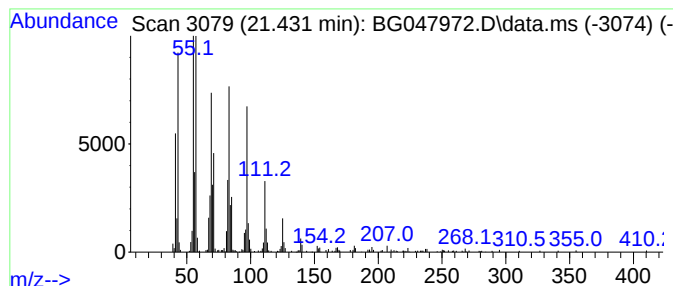
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.430	9.24 ng	421358	Chrysene-d12	21.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptacosanol	396	C27H56O	002004-39-9	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4			Behenic alcohol	326	C22H46O	000661-19-8	91
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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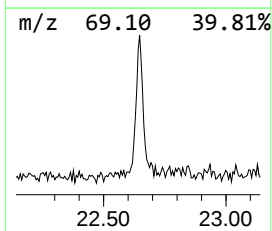
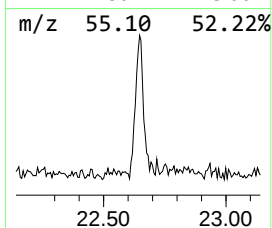
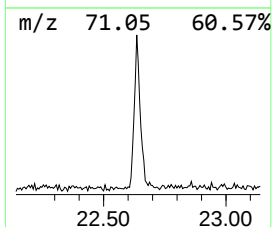
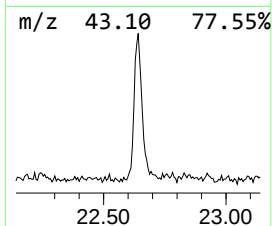
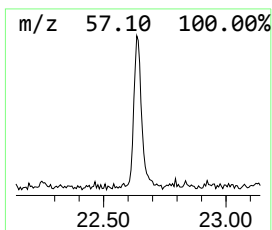
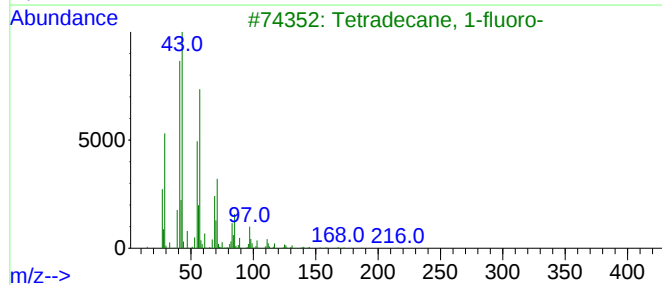
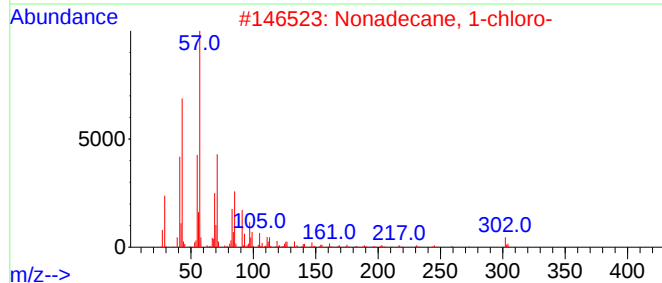
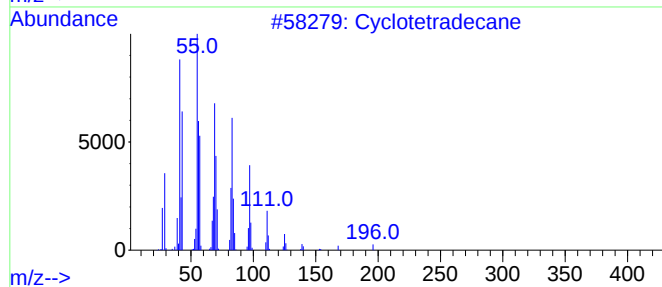
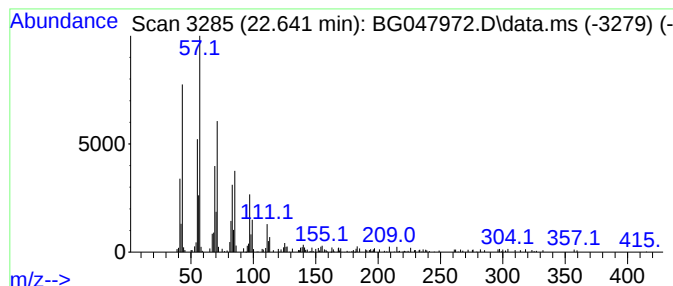
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Cyclotetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.641	6.04 ng	275398	Chrysene-d12	21.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	93
2			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	91
3			Tetradecane, 1-fluoro-	216	C14H29F	000593-33-9	90
4			Cyclododecane	168	C12H24	000294-62-2	80
5			Dodecane	170	C12H26	000112-40-3	78



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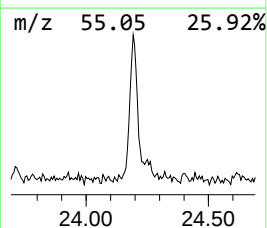
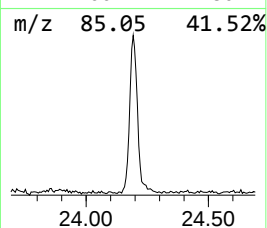
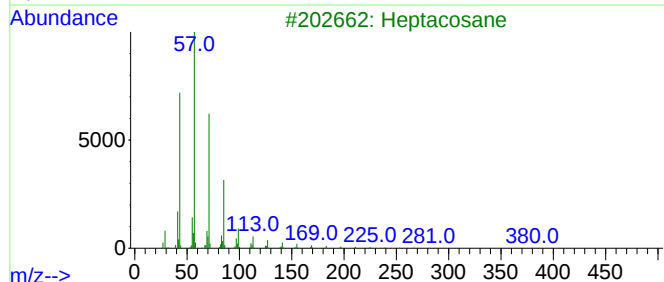
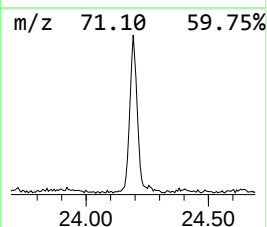
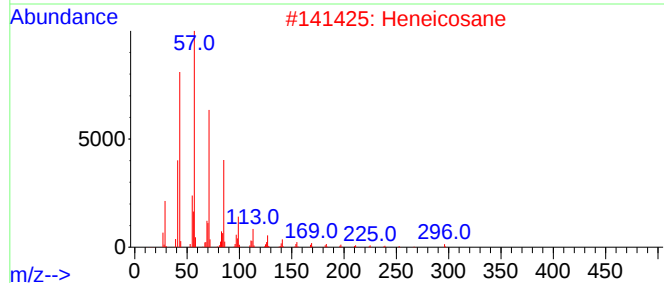
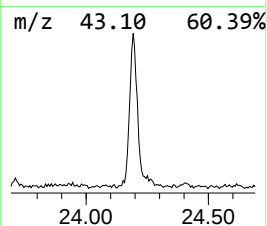
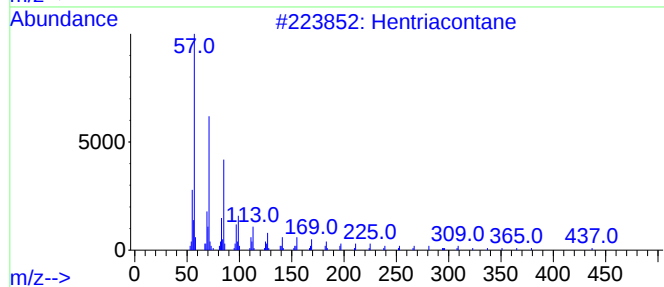
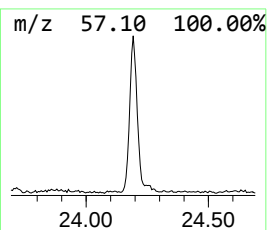
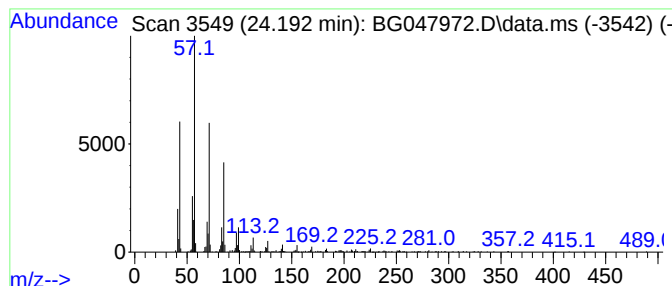
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hentriacontane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.192	13.01 ng	575801	Perylene-d12	25.103

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Octadecane	254	C18H38	000593-45-3	91
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91



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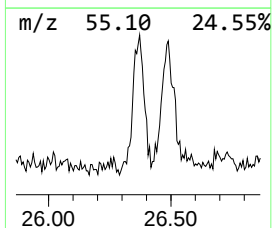
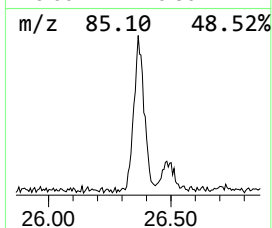
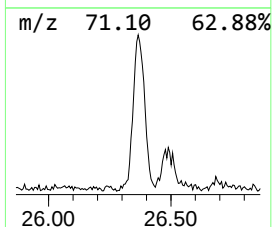
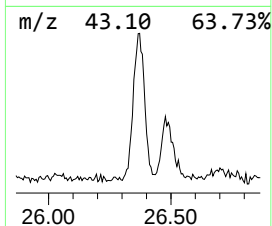
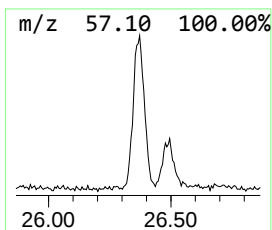
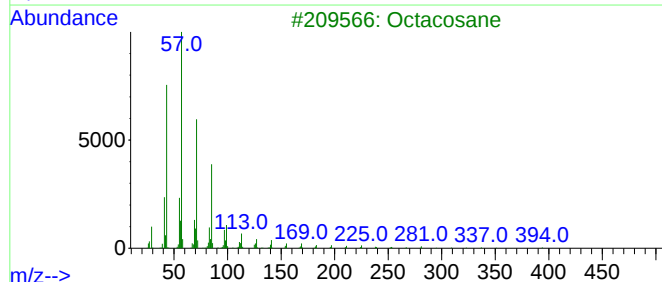
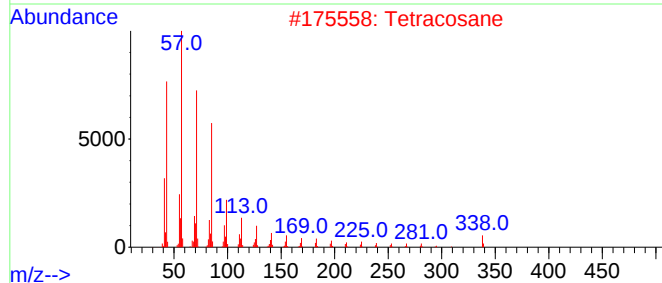
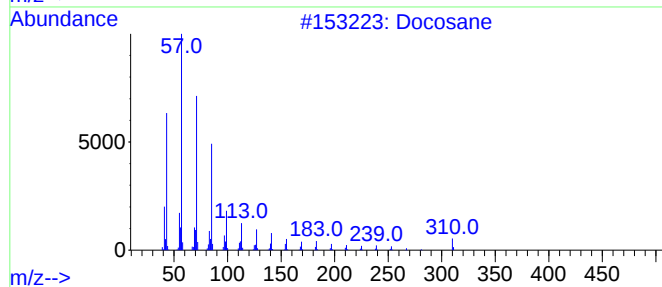
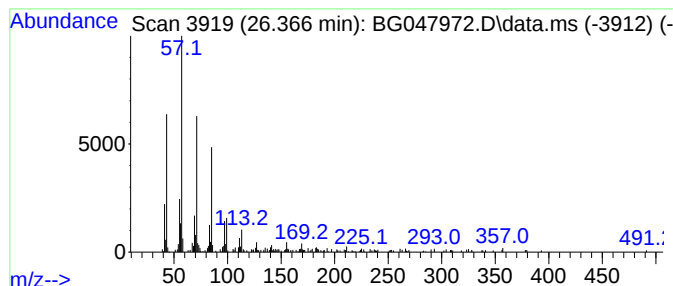
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Docosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.366	8.23 ng	364428	Perylene-d12	25.103

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane	310	C22H46	000629-97-0	93
2		Tetracosane	338	C24H50	000646-31-1	93
3		Octacosane	394	C28H58	000630-02-4	90
4		Hexacosane	366	C26H54	000630-01-3	90
5		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047972.D
Acq On : 22 Jan 2021 3:29
Operator : CG/JU
Sample : M1153-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-PS-01-068

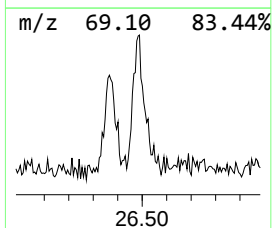
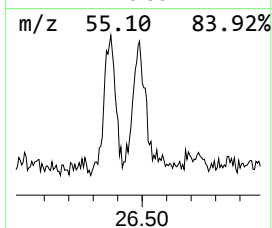
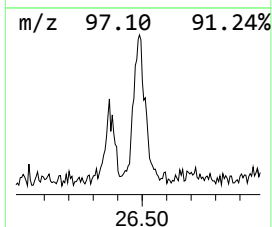
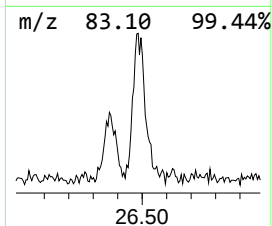
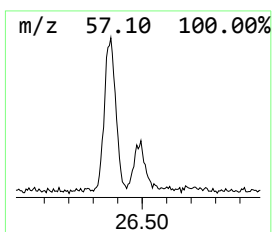
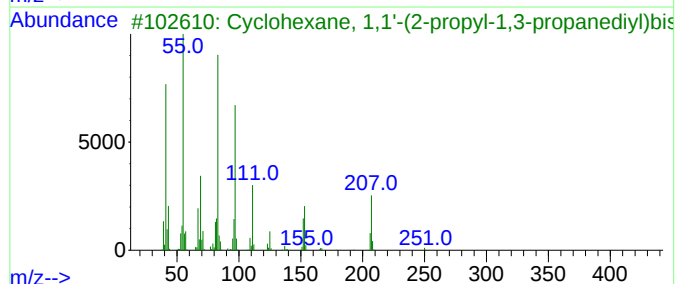
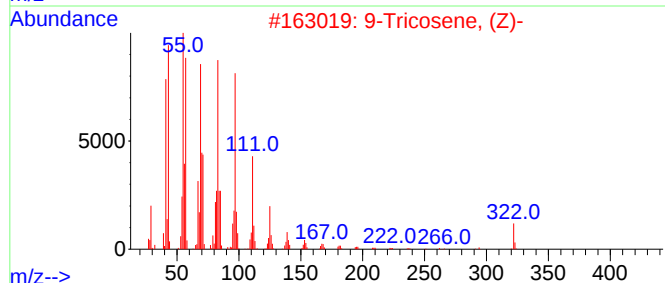
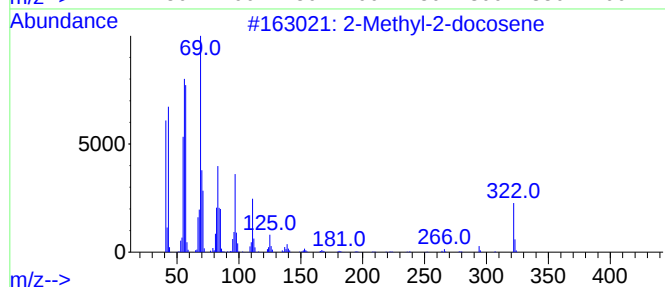
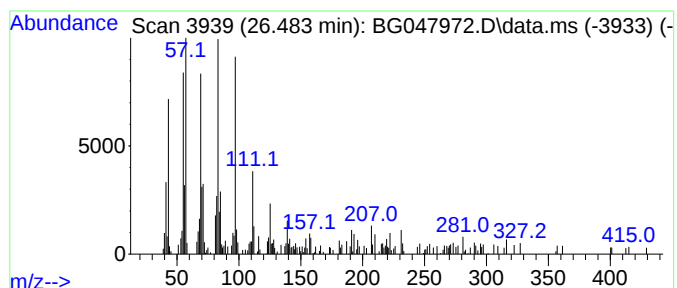
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Methyl-2-docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.483	5.64 ng	249742	Perylene-d12	25.103

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-2-docosene	322	C23H46	1000131-16-9	78
2			9-Tricosene, (Z)-	322	C23H46	027519-02-4	64
3			Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	60
4			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	58
5			1-Tetradecene	196	C14H28	001120-36-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047972.D
Acq On : 22 Jan 2021 3:29
Operator : CG/JU
Sample : M1153-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-PS-01-068

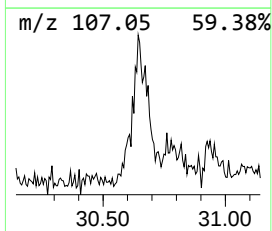
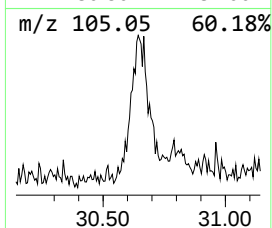
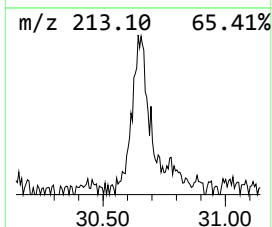
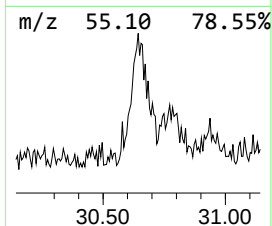
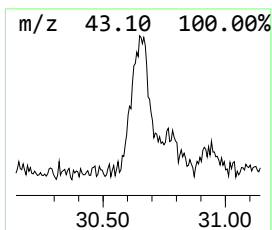
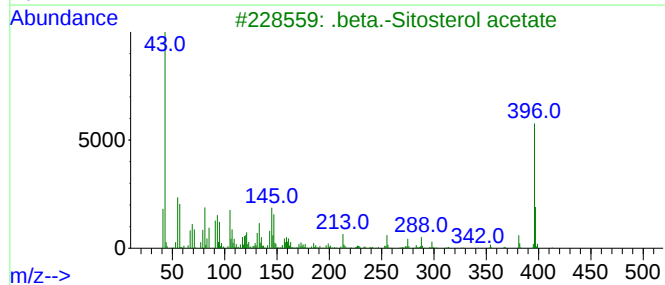
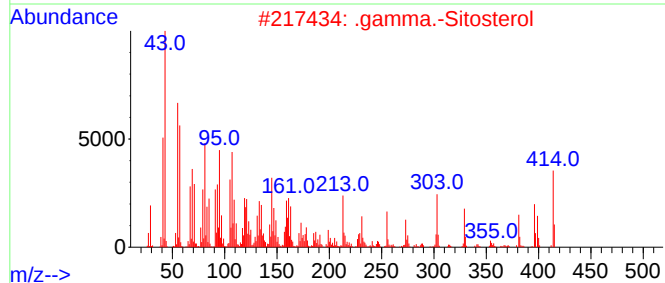
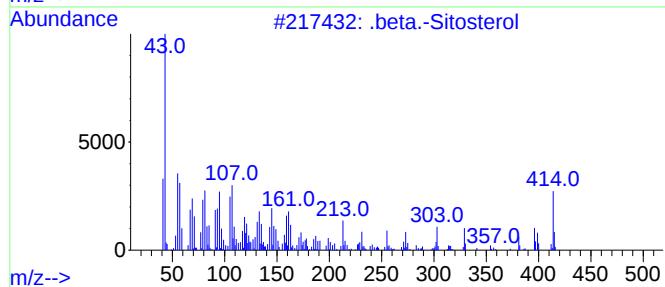
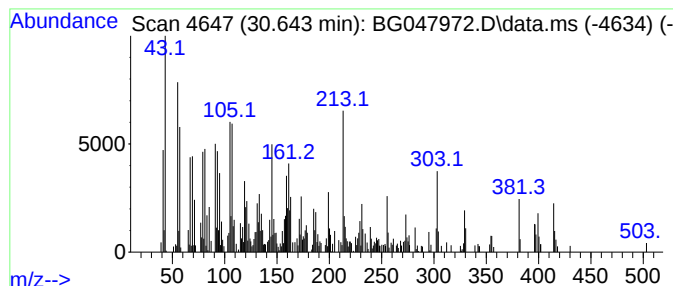
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown30.643 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.643	7.96 ng	352253	Perylene-d12	25.103

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-	Sitosterol	414	C29H50O	000083-46-5	49
2	.	gamma.-	Sitosterol	414	C29H50O	000083-47-6	46
3	.	beta.-	Sitosterol acetate	456	C31H52O2	000915-05-9	10
4			Ethinyl Estradiol	296	C20H24O2	000057-63-6	10
5			Acetic acid, 10,13-dimethyl-2-ox...	330	C21H30O3	1000190-79-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012121\
Data File : BG047972.D
Acq On : 22 Jan 2021 3:29
Operator : CG/JU
Sample : M1153-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FK-PS-01-068

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.393	8.4	ng	334052	4	17.512	794443	20.0
Octadecanoic acid	19.656	2.6	ng	118867	5	21.795	912184	20.0
1-Heptacosanol	21.430	9.2	ng	421358	5	21.795	912184	20.0
Cyclotetradecane	22.641	6.0	ng	275398	5	21.795	912184	20.0
Hentriacontane	24.192	13.0	ng	575801	6	25.103	885165	20.0
Docosane	26.366	8.2	ng	364428	6	25.103	885165	20.0
2-Methyl-2-doco...	26.483	5.6	ng	249742	6	25.103	885165	20.0
unknown30.643	30.643	8.0	ng	352253	6	25.103	885165	20.0