

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
 Data File : BF135195.D
 Acq On : 12 Sep 2023 22:37
 Operator : CG\JU
 Sample : 04335-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AREA-2

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_F\Methods\8270-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135195.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	11	16	22	rVB	33702	42204	1.25%	0.192%
2	5.016	493	498	507	rVB	66156	87473	2.60%	0.399%
3	5.399	559	563	566	rBV	2793305	2833636	84.14%	12.924%
4	6.404	729	734	737	rBV	2719613	2876492	85.41%	13.119%
5	6.763	791	795	798	rBV	778694	656835	19.50%	2.996%
6	7.328	885	891	894	rBV	1907447	1890274	56.13%	8.621%
7	8.040	1007	1012	1015	rBV	1046877	866923	25.74%	3.954%
8	9.122	1190	1196	1199	rBV	3660686	3343594	99.28%	15.249%
9	9.798	1305	1311	1314	rBV	1187467	986093	29.28%	4.497%
10	10.592	1441	1446	1449	rBV	2282977	2117853	62.88%	9.659%
11	11.286	1560	1564	1568	rBV	1215405	1081001	32.10%	4.930%
12	11.828	1652	1656	1668	rBV2	159813	195733	5.81%	0.893%
13	12.892	1831	1837	1840	rBV	3174279	3367937	100.00%	15.360%
14	13.822	1984	1995	2011	rBV3	82189	282718	8.39%	1.289%
15	13.939	2011	2015	2019	rBV	770934	694502	20.62%	3.167%
16	15.404	2259	2264	2277	rVB	489171	602951	17.90%	2.750%

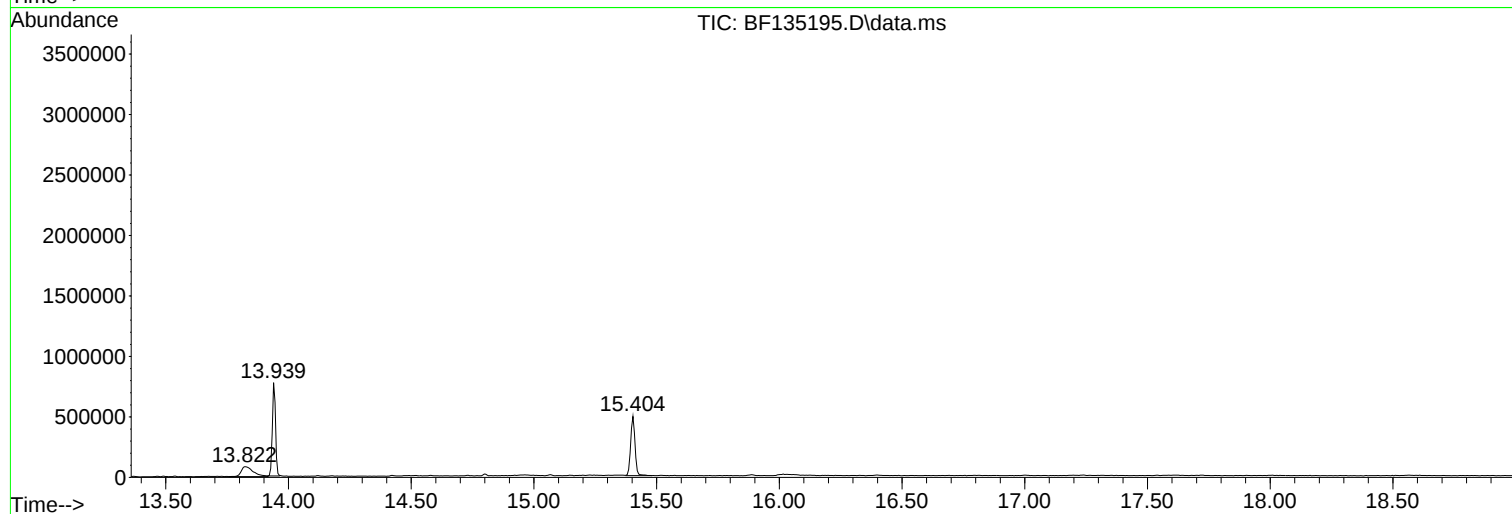
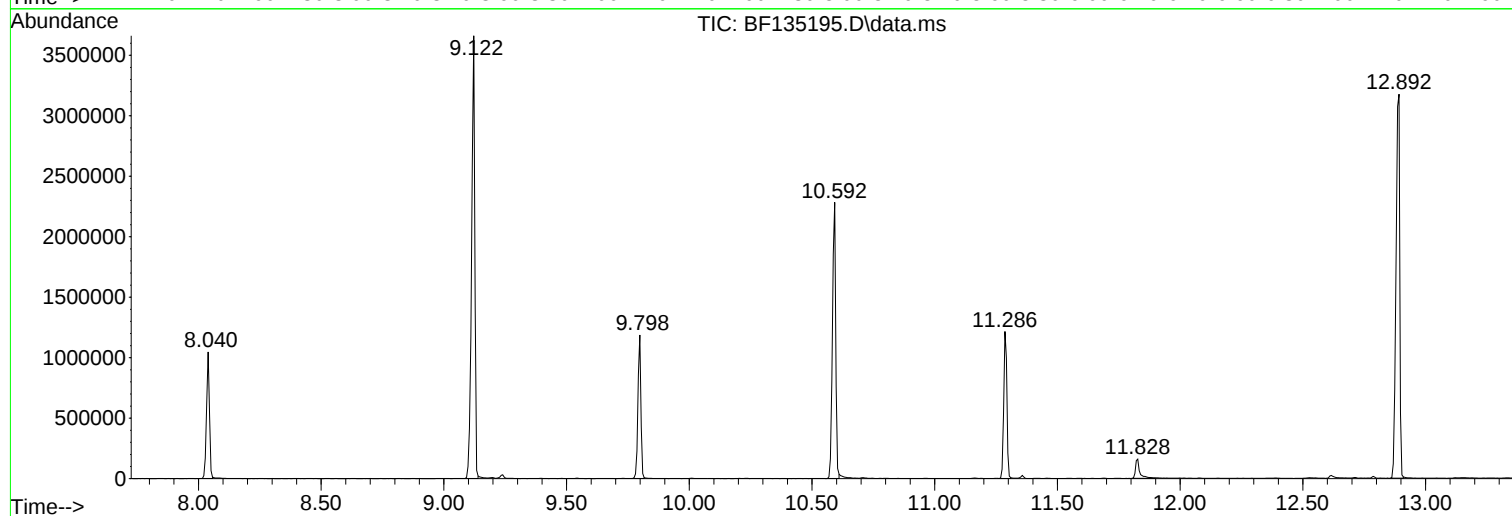
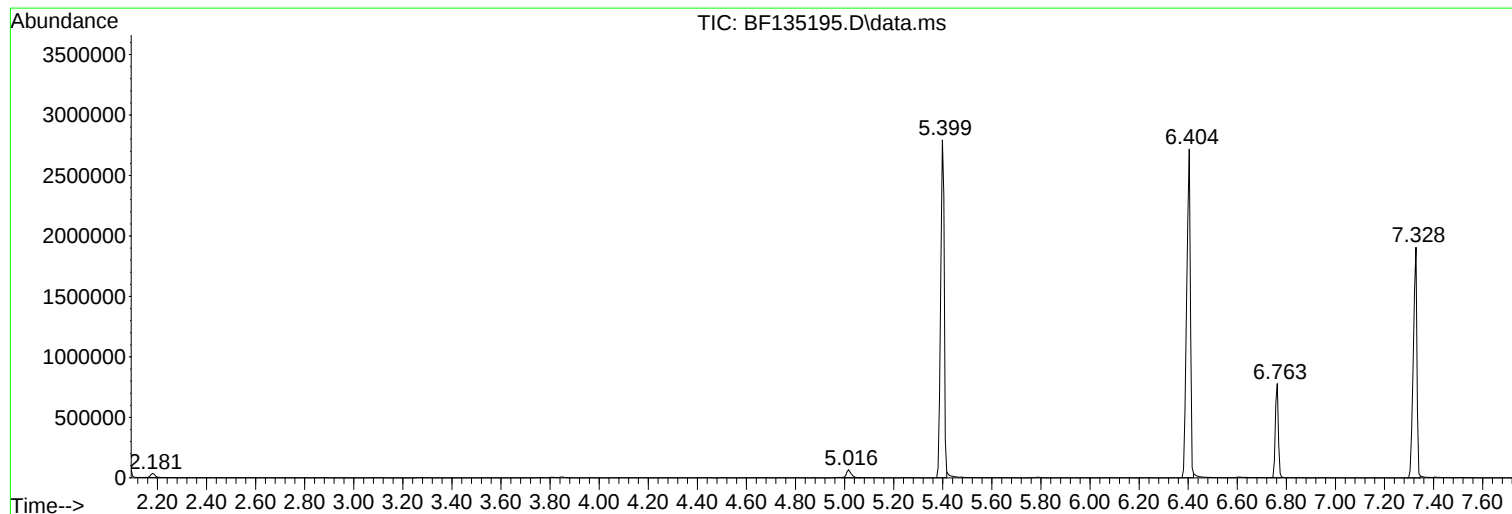
Sum of corrected areas: 21926219

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135195.D
Acq On : 12 Sep 2023 22:37
Operator : CG\JU
Sample : 04335-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AREA-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135195.D
Acq On : 12 Sep 2023 22:37
Operator : CG\JU
Sample : 04335-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AREA-2

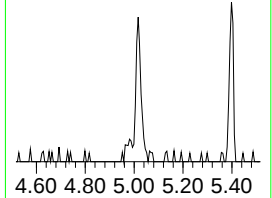
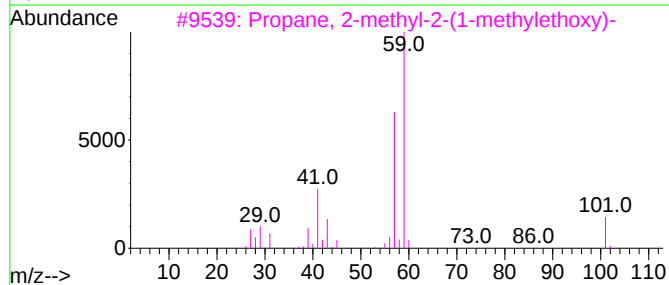
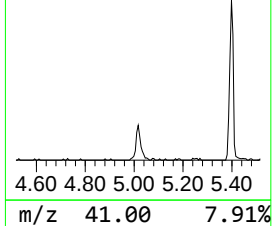
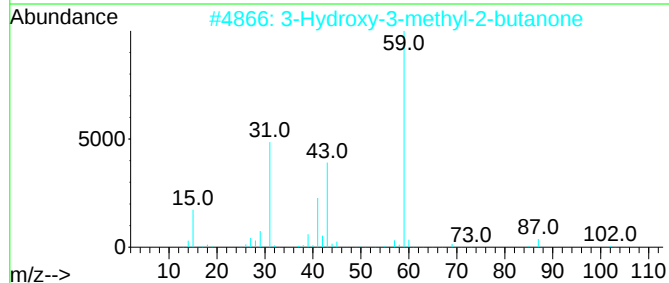
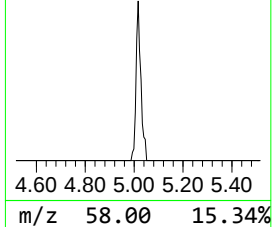
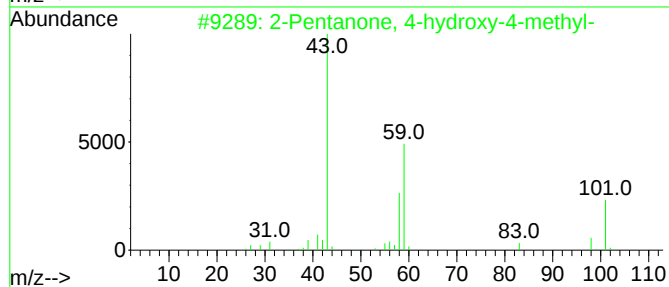
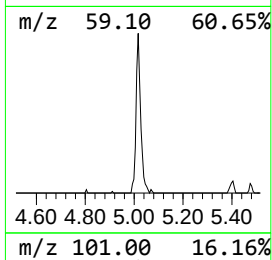
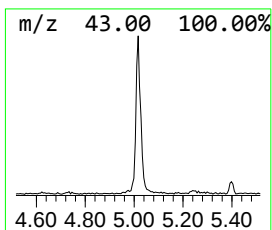
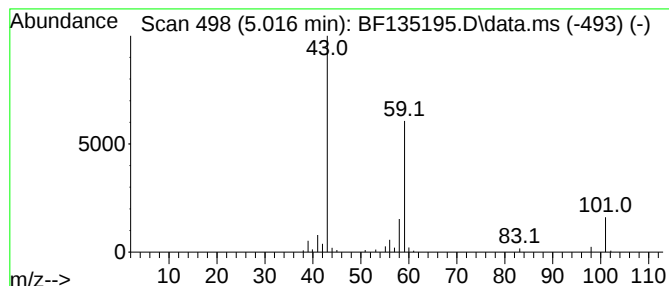
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.66 ng	87473	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135195.D
Acq On : 12 Sep 2023 22:37
Operator : CG\JU
Sample : 04335-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

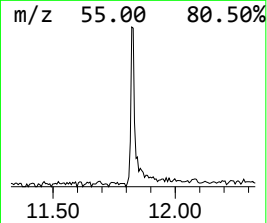
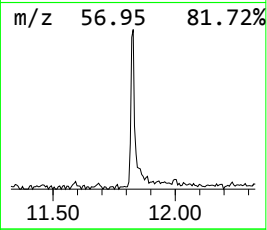
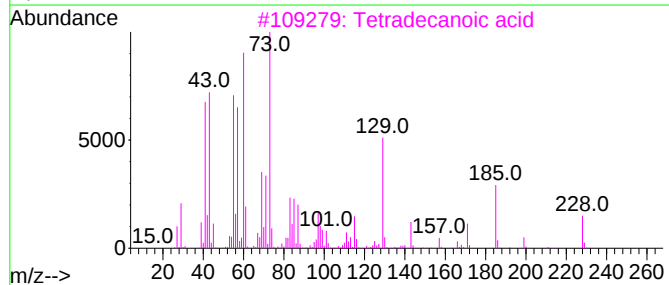
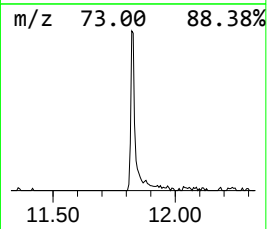
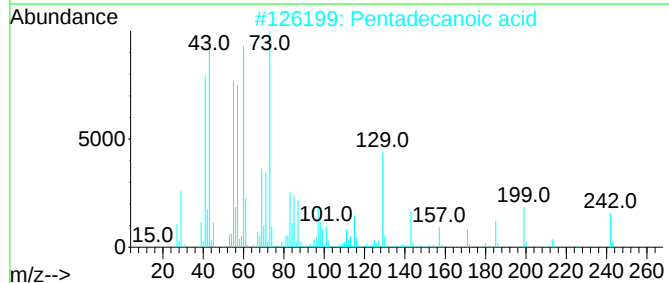
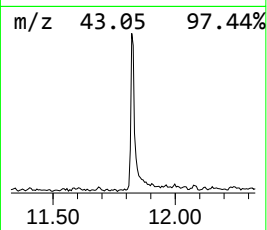
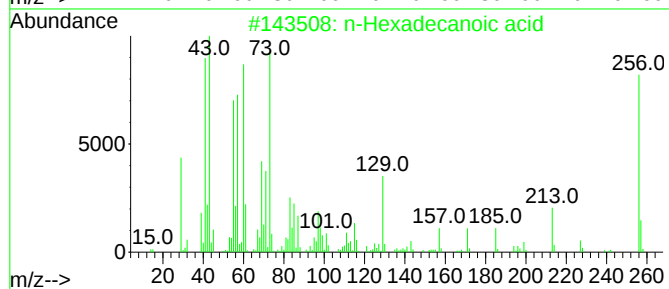
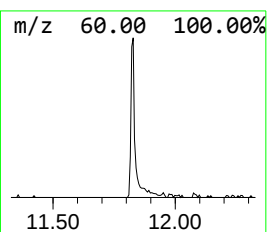
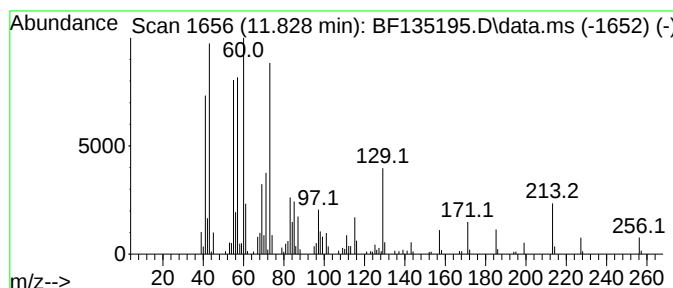
Instrument :
BNA_F
ClientSampleId :
AREA-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.828	3.62 ng	195733	Phenanthrene-d10		11.286	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
4	Tridecanoic acid		214	C13H26O2	000638-53-9	70
5	Dodecanoic acid		200	C12H24O2	000143-07-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135195.D
Acq On : 12 Sep 2023 22:37
Operator : CG\JU
Sample : 04335-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AREA-2

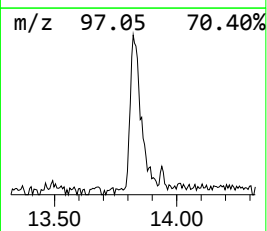
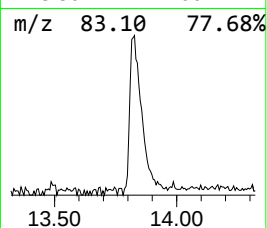
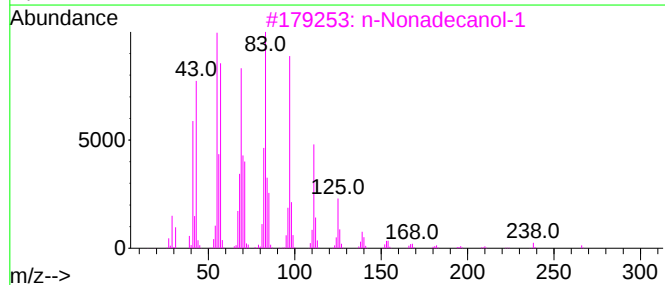
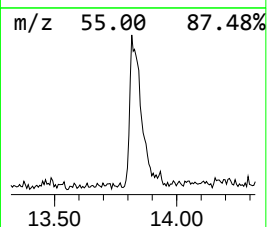
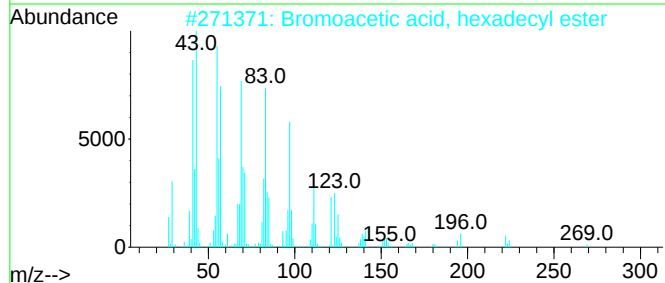
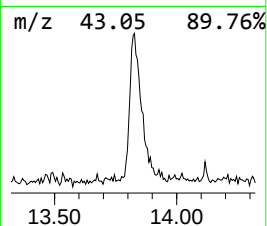
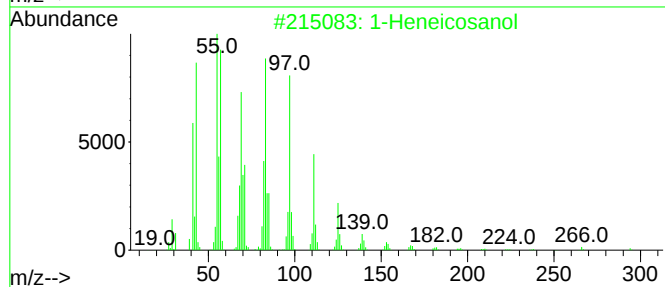
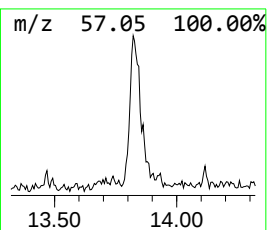
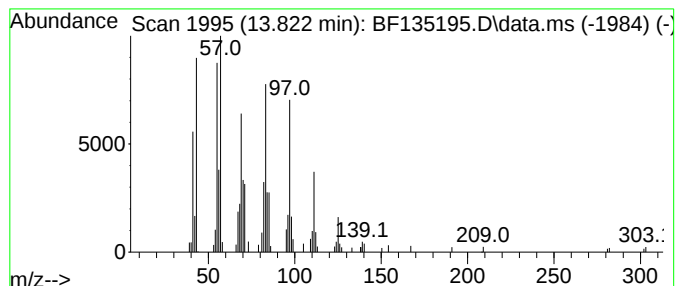
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Heneicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	8.14 ng	282718	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
4			1-Tricosene	322	C23H46	018835-32-0	91
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135195.D
Acq On : 12 Sep 2023 22:37
Operator : CG\JU
Sample : 04335-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AREA-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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-...	5.016	2.7	ng	87473	1	6.763	656835	20.0
n-Hexadecanoic ...	11.828	3.6	ng	195733	4	11.286	1081000	20.0
1-Heneicosanol	13.822	8.1	ng	282718	5	13.939	694502	20.0