

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
 Data File : BF122259.D
 Acq On : 4 Nov 2020 12:59
 Operator : JU/CG
 Sample : L4607-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OW-01

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-BF101220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.351	552	555	585	rBV	362646	947738	32.75%	4.947%
2	6.422	734	737	762	rBV2	217814	701546	24.24%	3.662%
3	6.598	762	767	776	rVV	16432	44122	1.52%	0.230%
4	6.710	783	786	796	rBV	473395	501862	17.34%	2.619%
5	7.281	879	883	899	rBV	1577629	1732370	59.86%	9.042%
6	7.992	1000	1004	1011	rBV	658353	655052	22.63%	3.419%
7	8.757	1131	1134	1141	rBV	29072	49664	1.72%	0.259%
8	9.069	1182	1187	1197	rBV	2739141	2894076	100.00%	15.106%
9	9.186	1203	1207	1214	rVB	325797	346002	11.96%	1.806%
10	9.469	1252	1255	1258	rVB	179189	151055	5.22%	0.788%
11	9.698	1291	1294	1297	rBV	63673	73962	2.56%	0.386%
12	9.745	1298	1302	1312	rVB	708513	755910	26.12%	3.946%
13	10.545	1434	1438	1452	rBV	1756621	1955367	67.56%	10.206%
14	11.233	1552	1555	1565	rBV	745397	738873	25.53%	3.857%
15	11.780	1644	1648	1654	rVB	850938	884924	30.58%	4.619%
16	12.563	1775	1781	1791	rVB	1031278	1288669	44.53%	6.726%
17	12.821	1821	1825	1828	rBV	2349503	2159380	74.61%	11.271%
18	13.721	1975	1978	1989	rVB	345372	465880	16.10%	2.432%
19	13.833	1992	1997	2003	rVV	351094	654889	22.63%	3.418%
20	13.886	2003	2006	2011	rVB	491624	478282	16.53%	2.496%
21	14.410	2090	2095	2101	rVB	310920	585698	20.24%	3.057%
22	14.692	2140	2143	2146	rVB	112356	117369	4.06%	0.613%
23	14.933	2179	2184	2191	rVB	271414	479872	16.58%	2.505%
24	15.327	2248	2251	2262	rVB	368878	496146	17.14%	2.590%

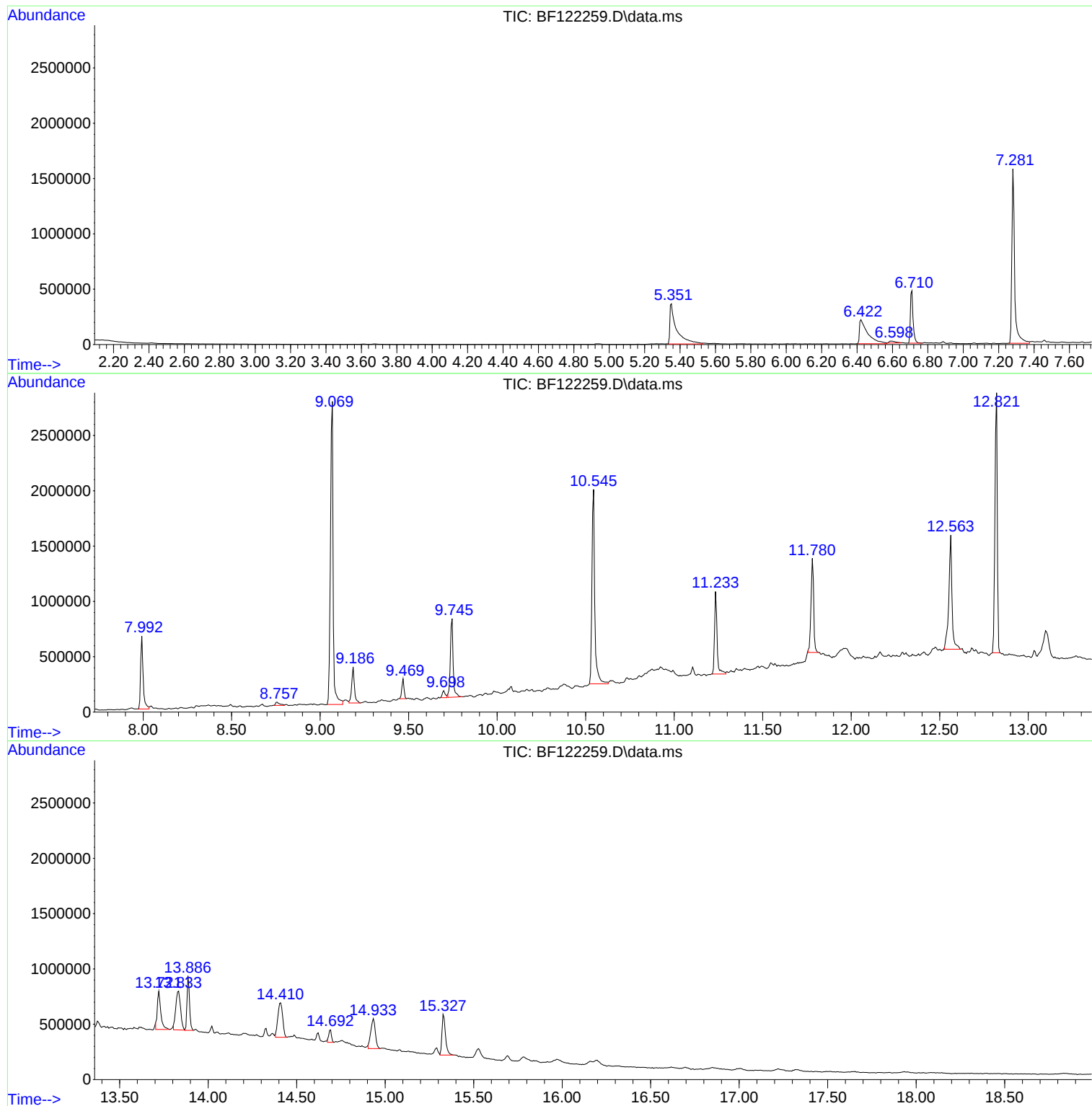
Sum of corrected areas: 19158708

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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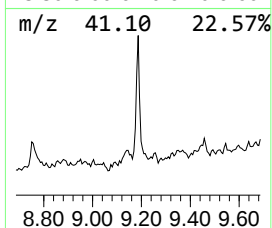
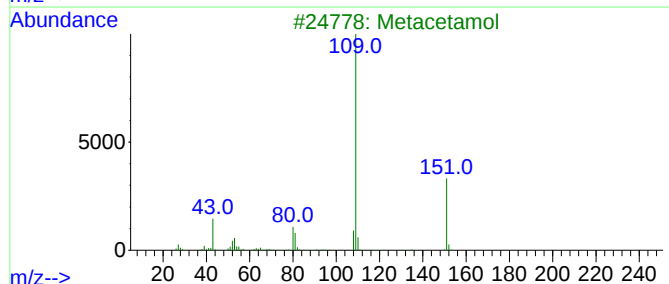
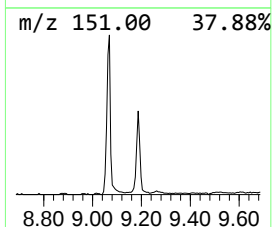
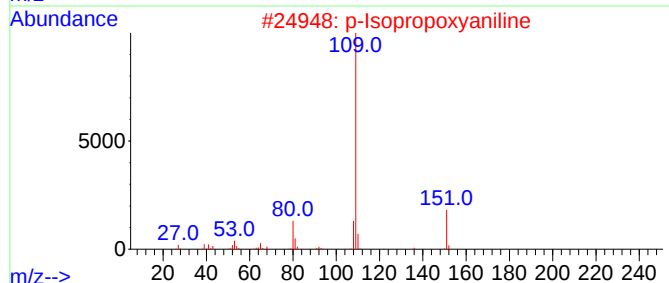
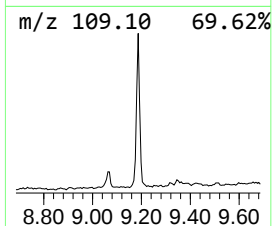
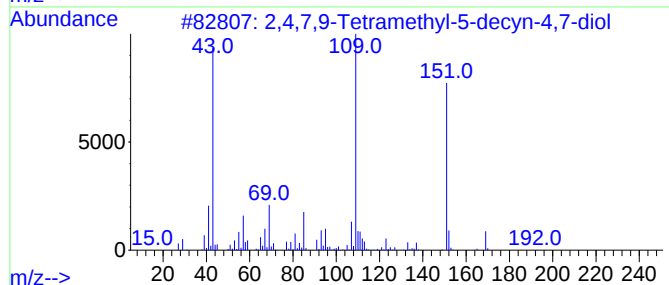
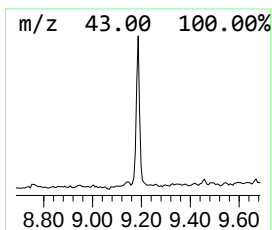
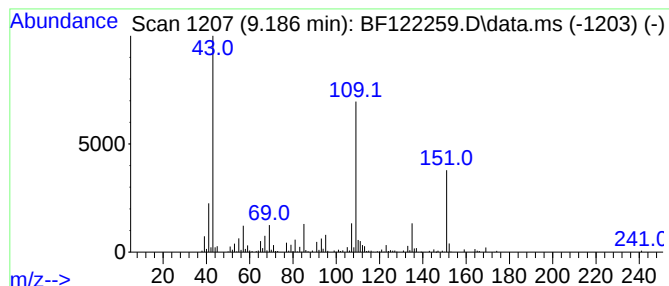
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.186	9.15 ng	346002	Acenaphthene-d10		9.745

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	72	
2	p-Isopropoxyaniline	151	C9H13NO	007664-66-6	46	
3	Metacetamol	151	C8H9NO2	000621-42-1	43	
4	Tiocarlide	400	C23H32N2O2S	000910-86-1	43	
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	43	



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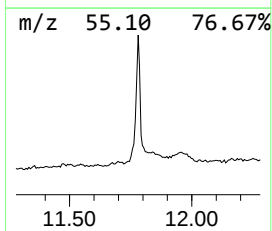
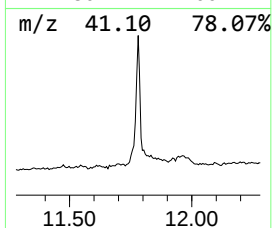
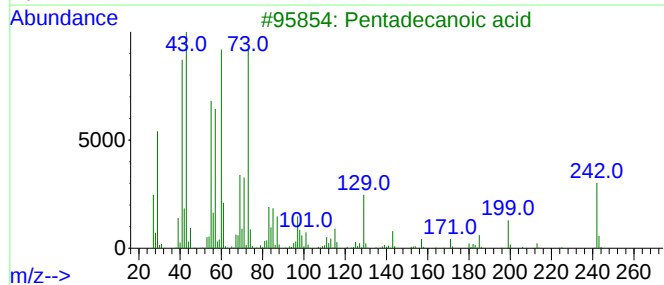
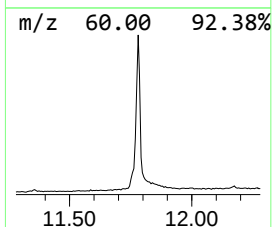
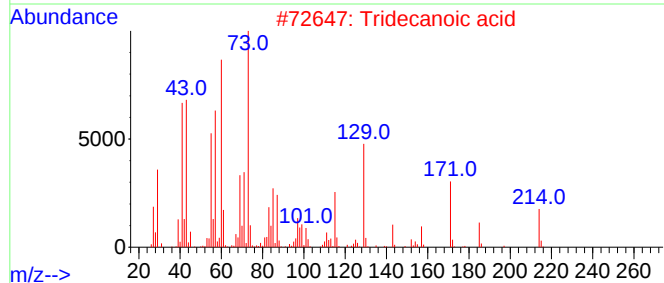
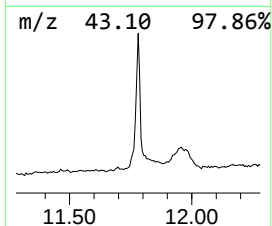
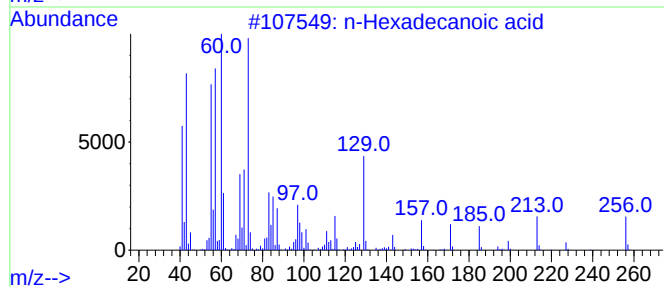
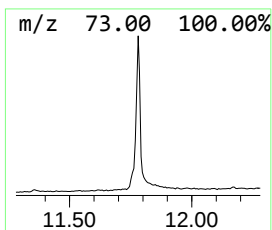
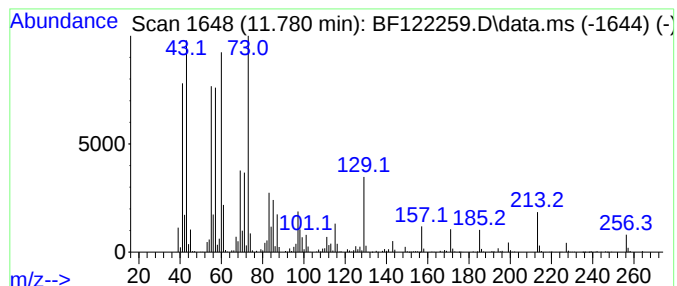
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	23.95 ng	884924	Phenanthrene-d10	11.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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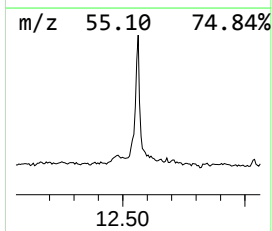
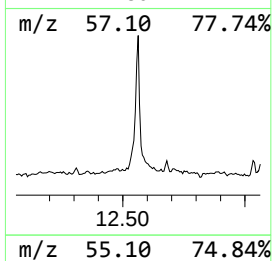
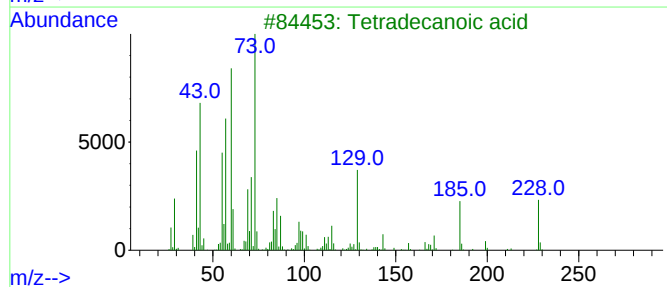
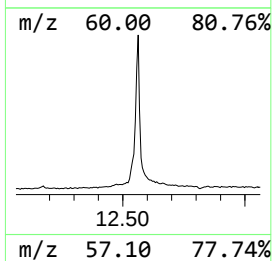
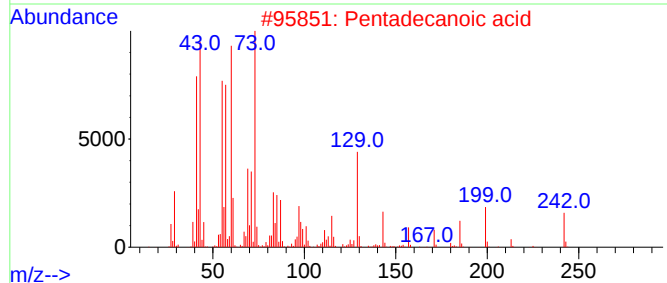
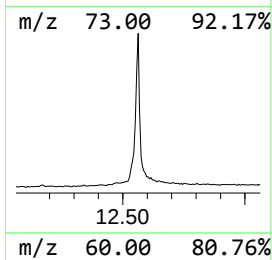
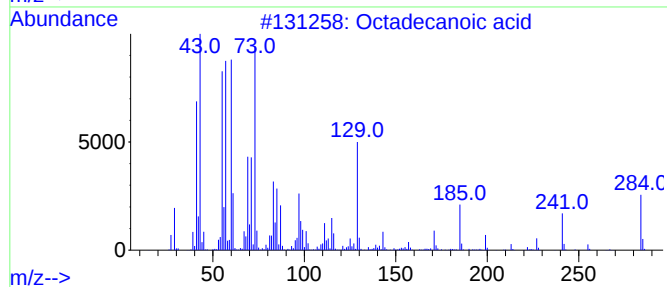
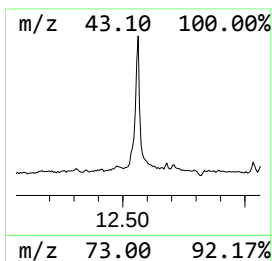
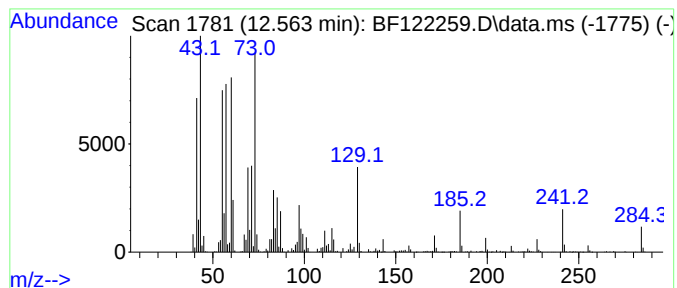
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Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	53.89 ng	1288670	Chrysene-d12	13.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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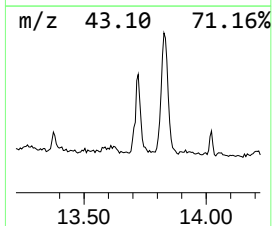
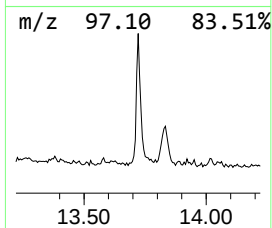
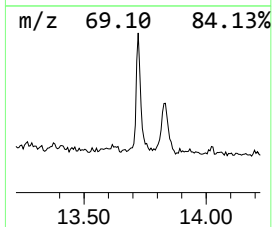
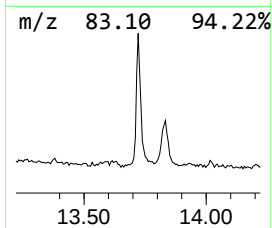
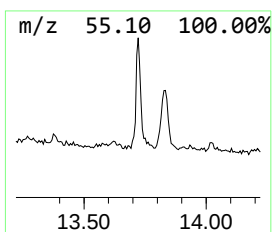
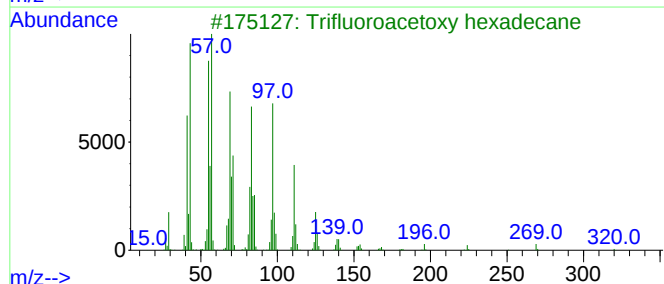
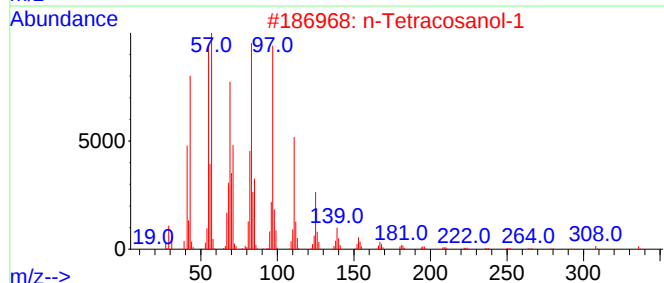
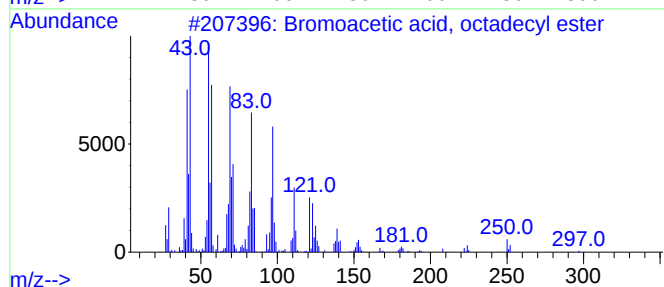
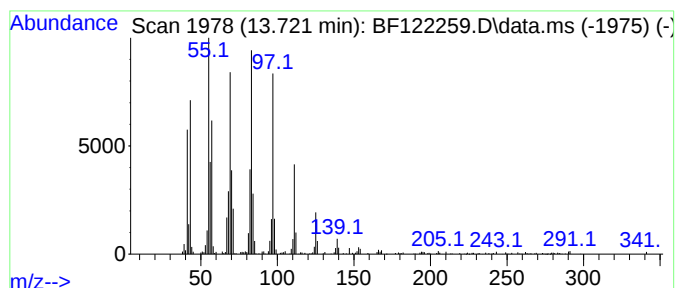
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.721	19.48 ng	465880	Chrysene-d12		13.886	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester		390	C20H39BrO2	018992-03-5	91
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	91
3	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	90
4	1-Heneicosanol		312	C21H44O	015594-90-8	90
5	1-Hexadecanol		242	C16H34O	036653-82-4	81



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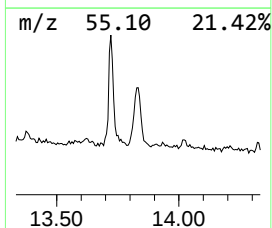
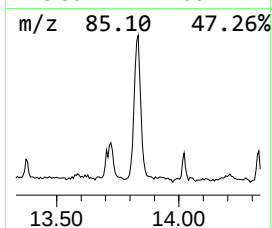
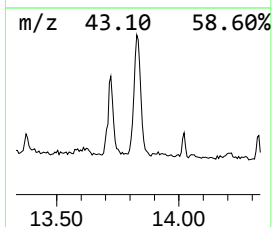
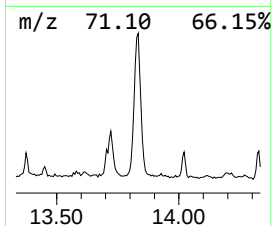
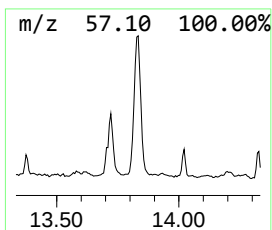
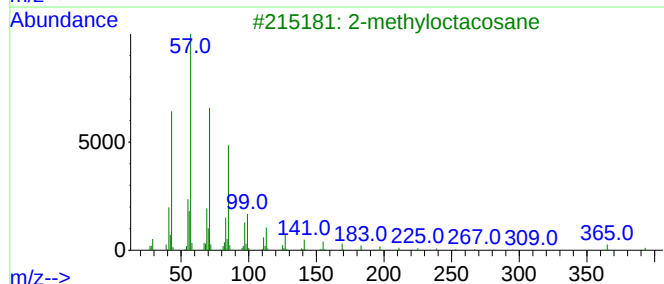
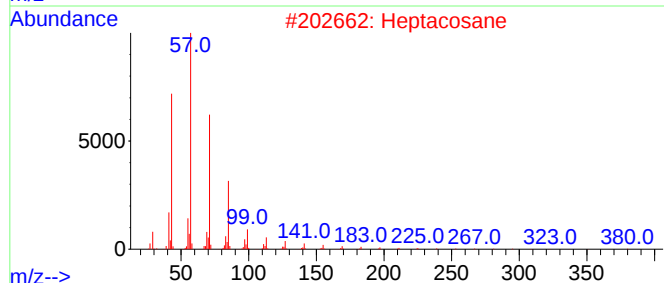
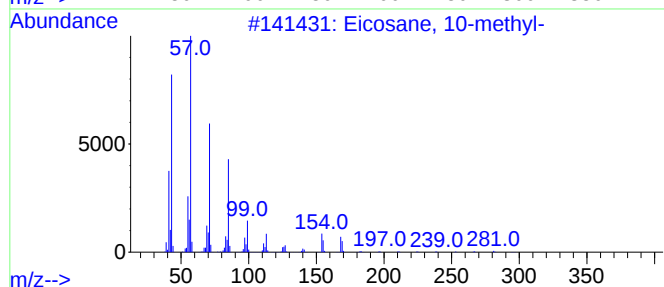
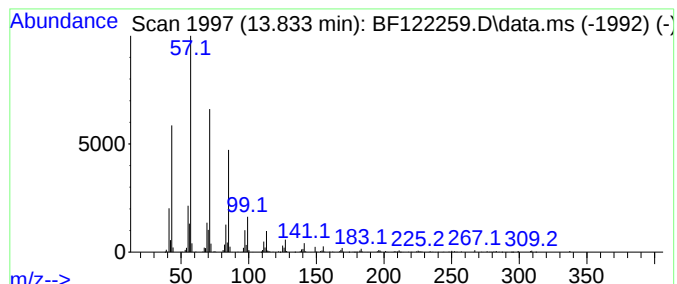
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane, 10-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.833	27.39 ng	654889	Chrysene-d12	13.886	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2	Heptacosane	380	C27H56	000593-49-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
5	Tetratetracontane	619	C44H90	007098-22-8	83



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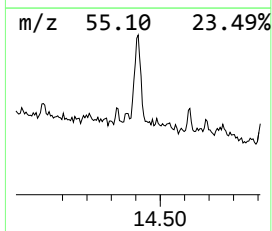
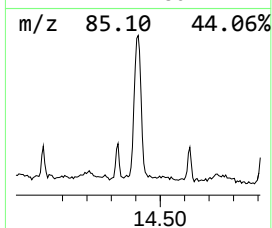
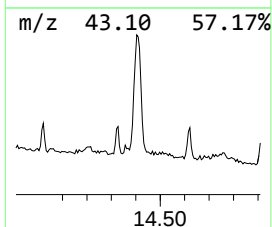
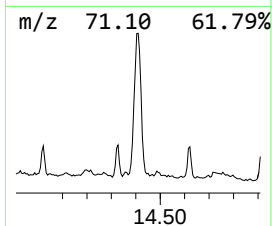
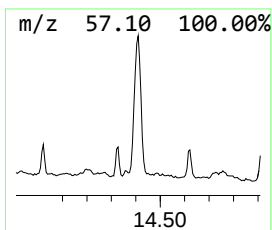
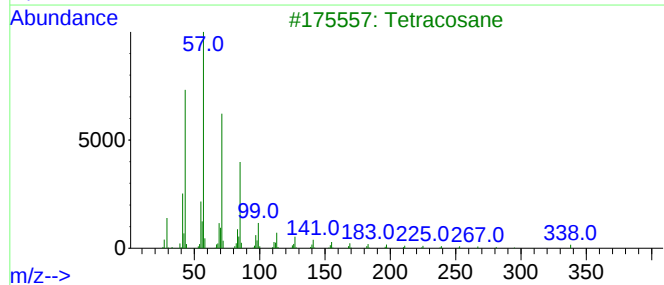
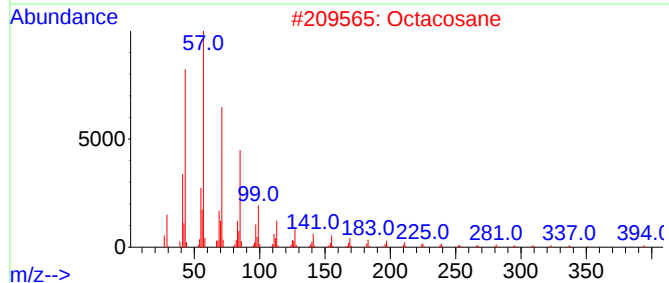
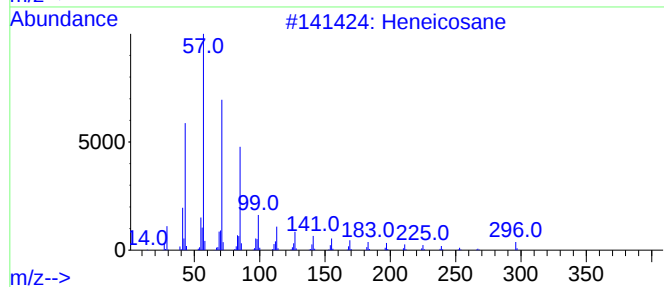
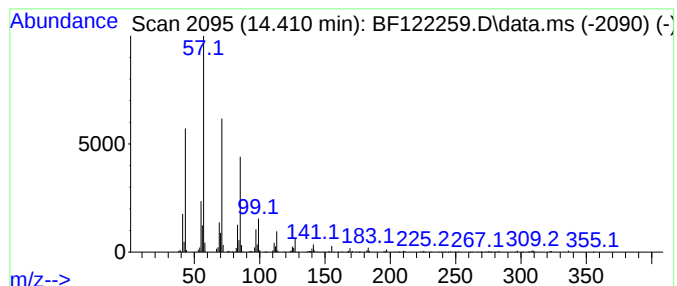
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.410	24.49 ng	585698	Chrysene-d12	13.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Octacosane	394	C28H58	000630-02-4	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122259.D
Acq On : 4 Nov 2020 12:59
Operator : JU/CG
Sample : L4607-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

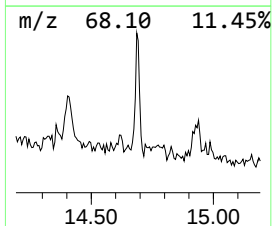
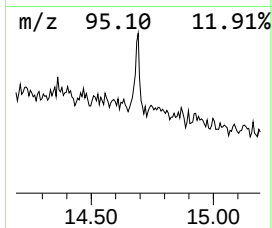
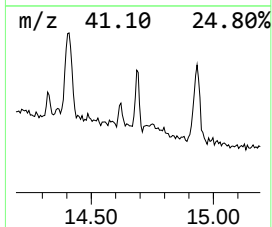
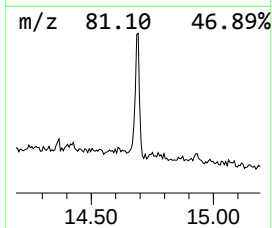
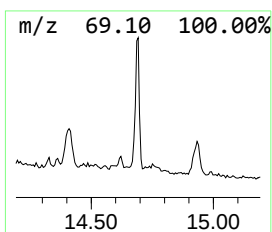
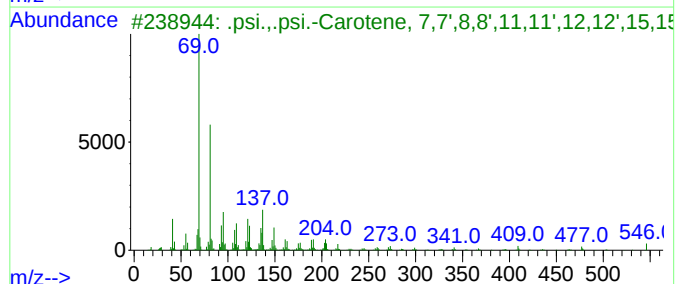
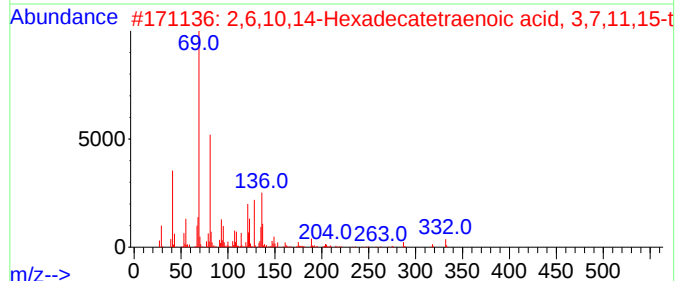
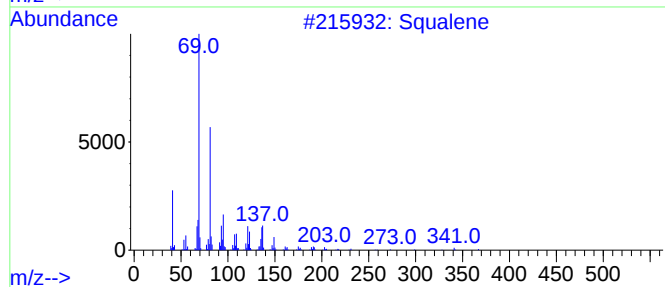
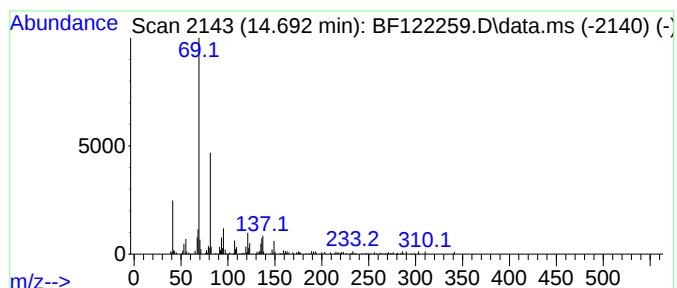
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.692	4.73 ng	117369	Perylene-d12	15.327	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	87
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122259.D
Acq On : 4 Nov 2020 12:59
Operator : JU/CG
Sample : L4607-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OW-01

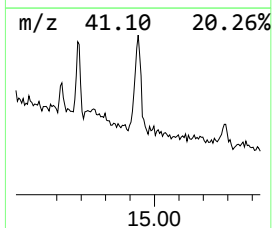
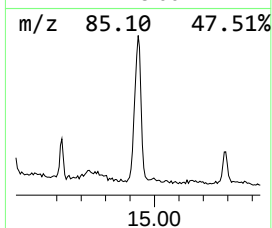
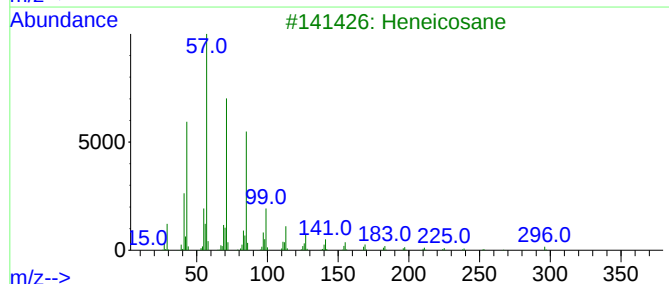
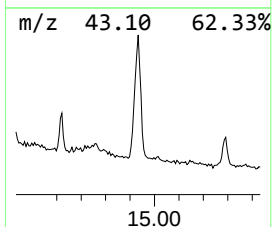
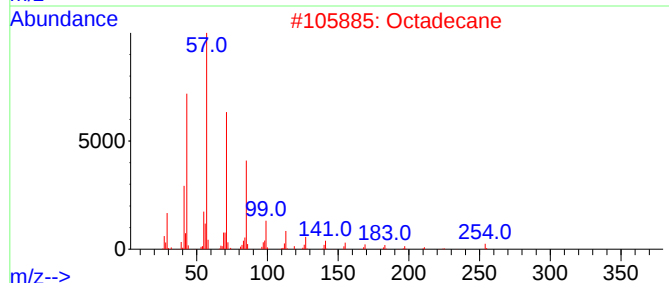
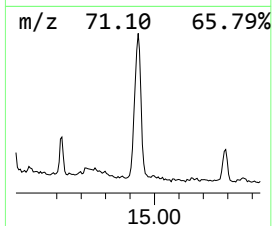
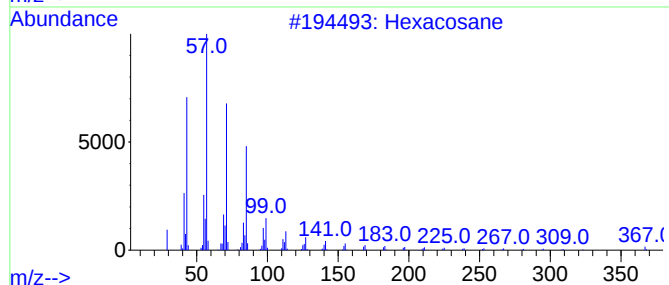
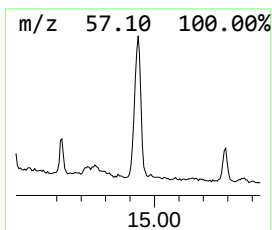
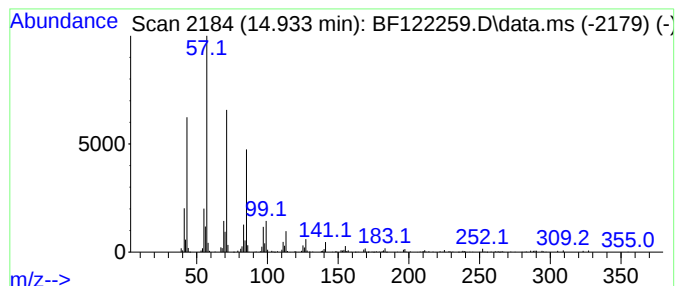
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	19.34 ng	479872	Perylene-d12	15.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	94
2			Octadecane	254	C18H38	000593-45-3	93
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110420\
Data File : BF122259.D
Acq On : 4 Nov 2020 12:59
Operator : JU/CG
Sample : L4607-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
2,4,7,9-Tetrame...	9.186	9.2	ng	346002	3	9.745	755910	20.0
n-Hexadecanoic ...	11.780	23.9	ng	884924	4	11.233	738873	20.0
Octadecanoic acid	12.563	53.9	ng	1288670	5	13.886	478282	20.0
Bromoacetic aci...	13.721	19.5	ng	465880	5	13.886	478282	20.0
Eicosane, 10-me...	13.833	27.4	ng	654889	5	13.886	478282	20.0
Heneicosane	14.410	24.5	ng	585698	5	13.886	478282	20.0
Squalene	14.692	4.7	ng	117369	6	15.327	496146	20.0
Hexacosane	14.933	19.3	ng	479872	6	15.327	496146	20.0