

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
 Data File : BF136918.D
 Acq On : 03 Jan 2024 20:51
 Operator : CG\JU
 Sample : 05897-17
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-21

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136918.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	494	498	504	rVB	20733	26015	2.32%	0.263%
2	5.422	564	567	585	rBV	1218102	1121410	100.00%	11.320%
3	6.428	734	738	754	rBV	1210748	1095440	97.68%	11.058%
4	6.781	794	798	802	rBV	477808	364008	32.46%	3.674%
5	7.339	889	893	896	rBV	789248	734169	65.47%	7.411%
6	8.057	1011	1015	1018	rBV	624542	484331	43.19%	4.889%
7	8.769	1133	1136	1140	rVB	17494	14375	1.28%	0.145%
8	9.133	1194	1198	1201	rBV	1409449	1073277	95.71%	10.834%
9	9.810	1310	1313	1317	rBV	610388	535200	47.73%	5.402%
10	9.910	1326	1330	1336	rBV5	9331	13614	1.21%	0.137%
11	10.604	1444	1448	1460	rVB	713217	626870	55.90%	6.328%
12	10.733	1465	1470	1473	rVB2	15210	17336	1.55%	0.175%
13	11.304	1563	1567	1571	rBV	609864	506003	45.12%	5.108%
14	11.569	1607	1612	1615	rBV7	7013	13595	1.21%	0.137%
15	11.839	1654	1658	1670	rBV	242733	248747	22.18%	2.511%
16	12.392	1746	1752	1764	rBV3	53928	142644	12.72%	1.440%
17	12.527	1772	1775	1777	rBV	17846	17249	1.54%	0.174%
18	12.627	1789	1792	1801	rBV	72696	89769	8.01%	0.906%
19	12.898	1834	1838	1842	rBV	925375	769417	68.61%	7.767%
20	13.127	1873	1877	1880	rBV3	24367	30734	2.74%	0.310%
21	13.474	1931	1936	1938	rBV2	22904	24911	2.22%	0.251%
22	13.810	1989	1993	1995	rBV	91728	85325	7.61%	0.861%
23	13.839	1995	1998	2011	rVB3	44552	103329	9.21%	1.043%
24	13.963	2011	2019	2027	rBV	393139	409984	36.56%	4.138%
25	14.027	2027	2030	2033	rBV4	12290	16210	1.45%	0.164%
26	14.127	2043	2047	2050	rVB	23183	24256	2.16%	0.245%
27	14.433	2095	2099	2103	rBV	111282	106210	9.47%	1.072%
28	14.486	2103	2108	2112	rBV6	40446	79844	7.12%	0.806%
29	14.739	2146	2151	2154	rVB4	21061	27718	2.47%	0.280%
30	14.892	2174	2177	2180	rVB5	13717	14338	1.28%	0.145%
31	15.080	2206	2209	2214	rVB	60453	69162	6.17%	0.698%
32	15.163	2217	2223	2237	rBV3	72011	210397	18.76%	2.124%
33	15.380	2257	2260	2265	rVB5	12660	15889	1.42%	0.160%
34	15.445	2266	2271	2279	rVB	297991	417762	37.25%	4.217%
35	15.674	2307	2310	2315	rVB4	20036	27341	2.44%	0.276%
36	15.915	2347	2351	2356	rVB2	42292	57298	5.11%	0.578%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.039	2365	2372	2386	rBV6	56052	215299	19.20%	2.173%
38	16.980	2526	2532	2538	rVB9	19476	43883	3.91%	0.443%
39	17.051	2540	2544	2550	rVB4	19597	33372	2.98%	0.337%

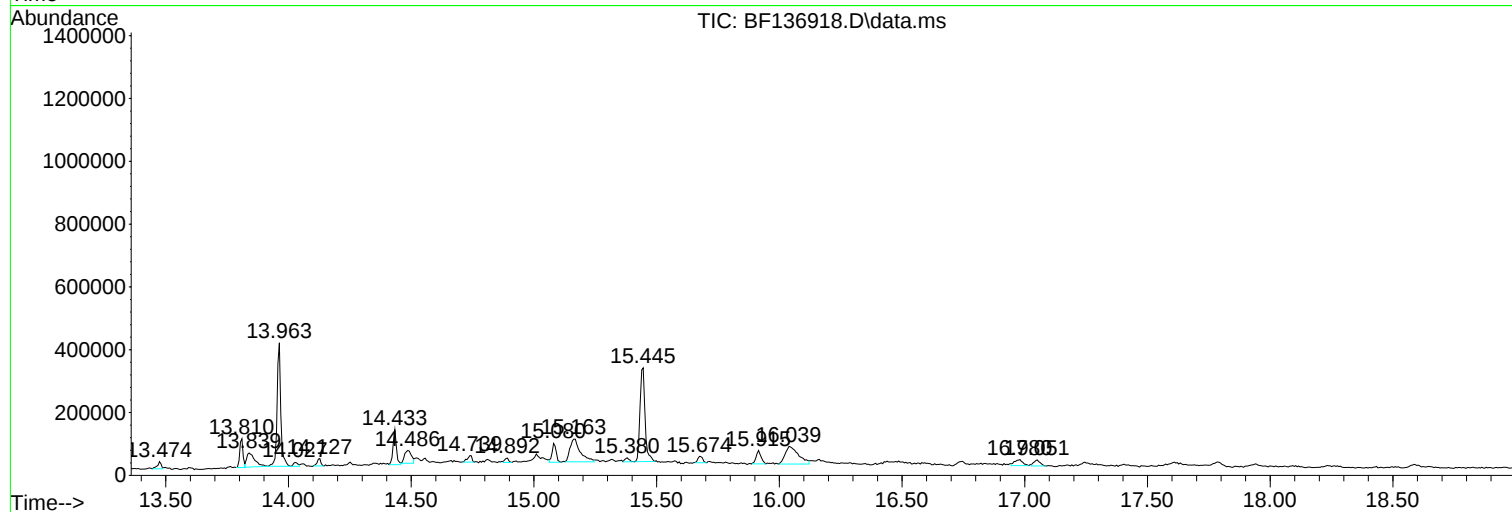
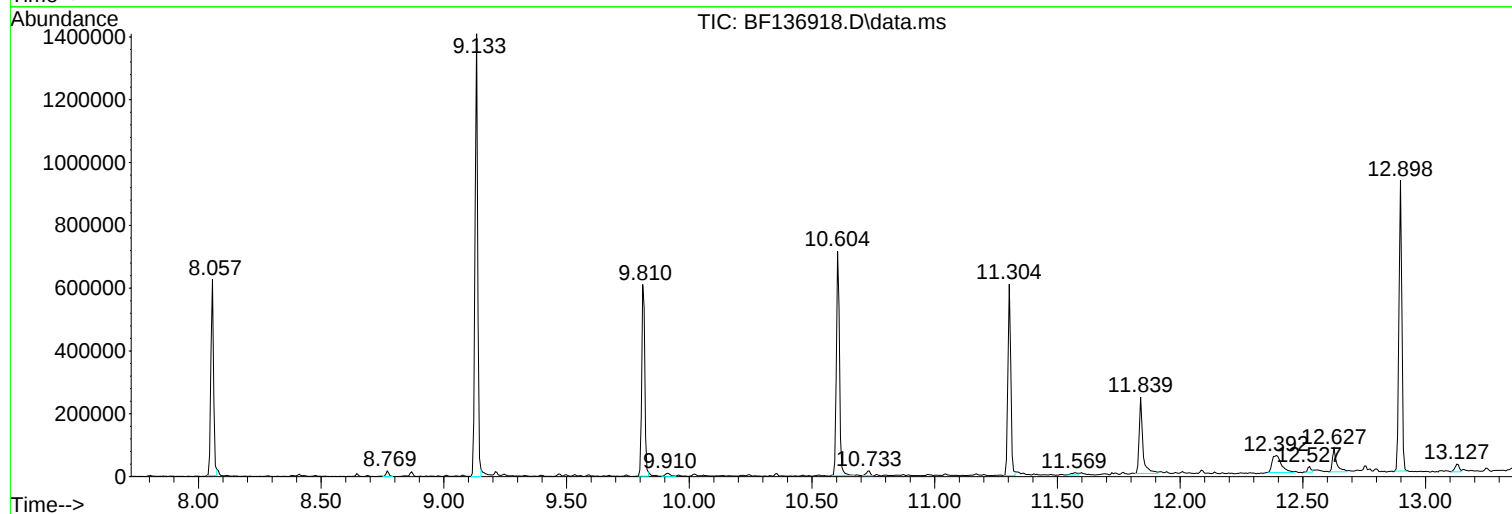
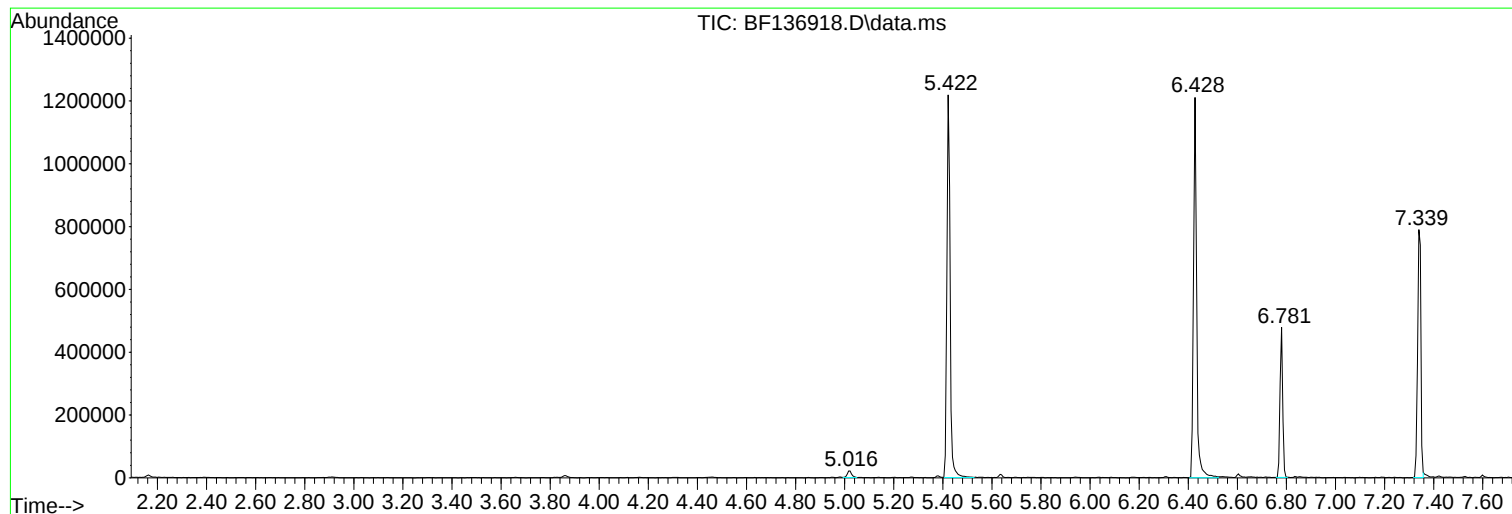
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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BNA_F
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GHL-SS-21

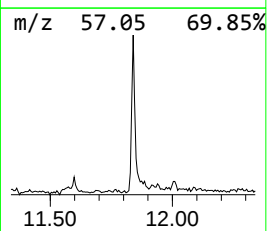
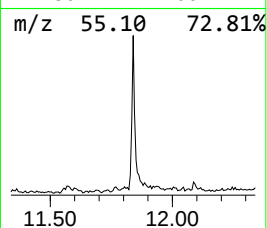
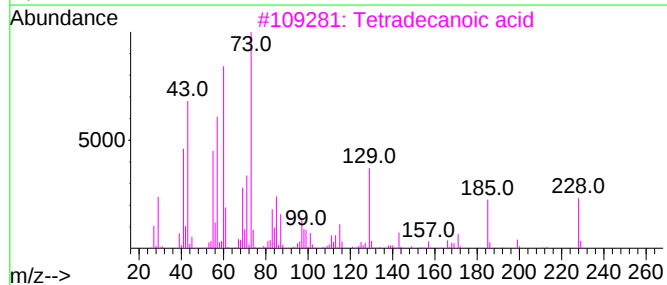
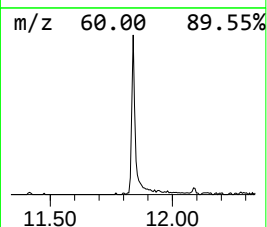
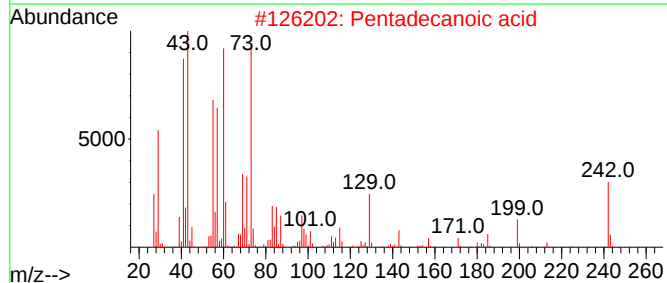
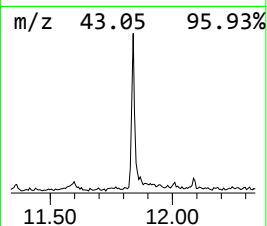
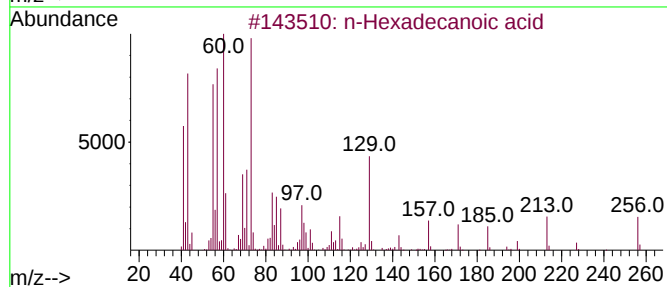
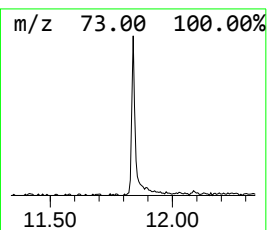
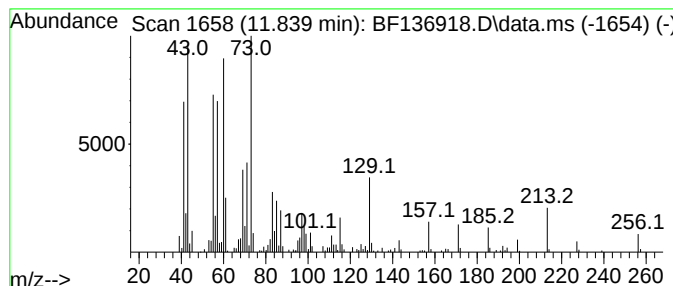
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	9.83 ng	248747	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	68
5			Octanoic acid	144	C8H16O2	000124-07-2	46



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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-21

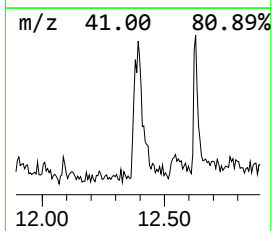
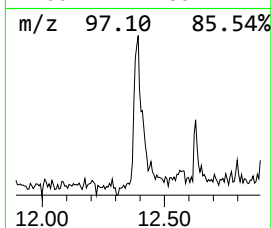
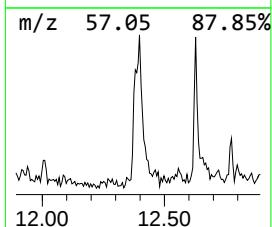
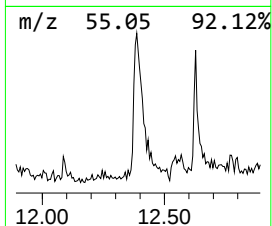
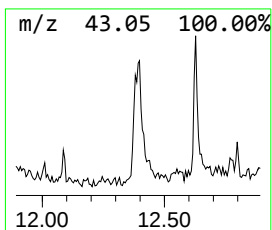
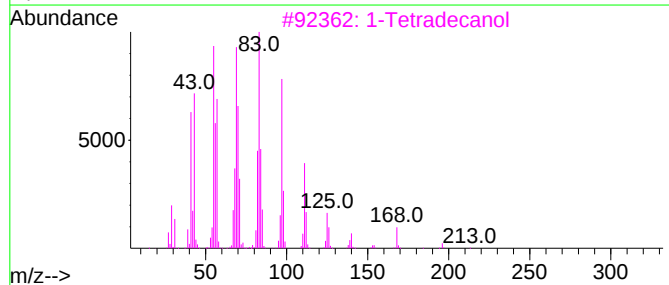
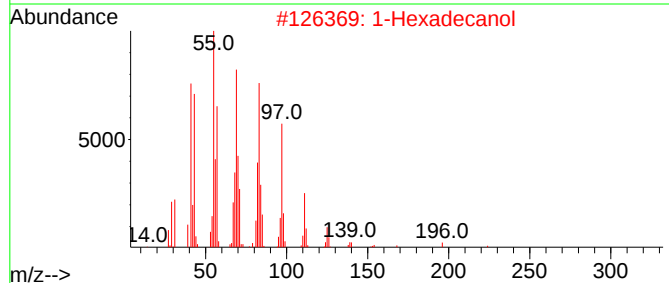
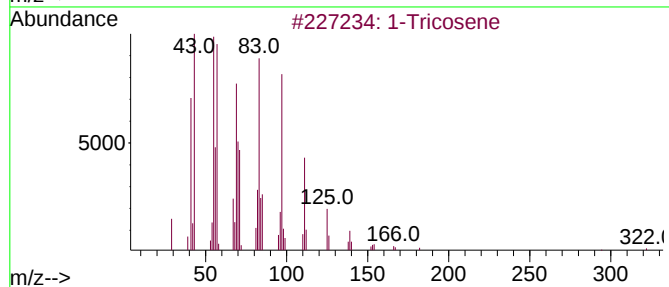
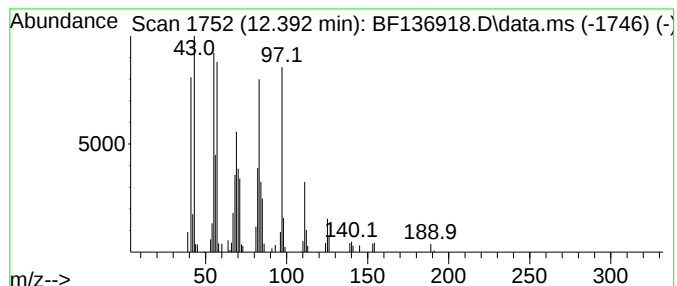
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.392	5.64 ng	142644	Phenanthrene-d10	11.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene		322	C23H46	018835-32-0	90
2	1-Hexadecanol		242	C16H34O	036653-82-4	83
3	1-Tetradecanol		214	C14H30O	000112-72-1	83
4	Trichloroacetic acid, tetradecyl...		358	C16H29Cl3O2	074339-52-9	81
5	1-Octadecene		252	C18H36	000112-88-9	81



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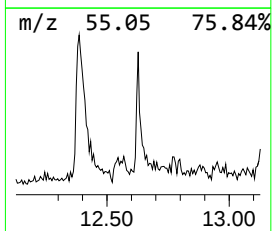
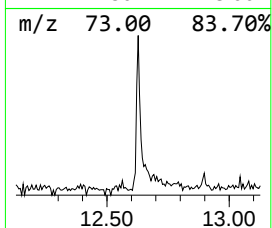
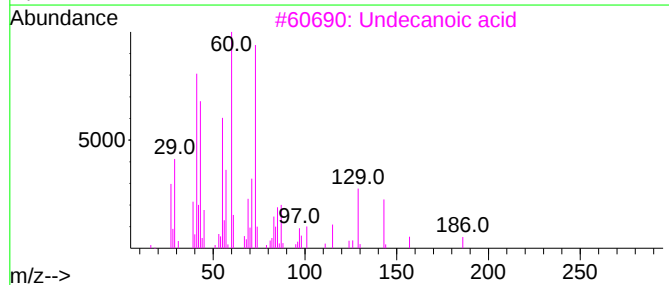
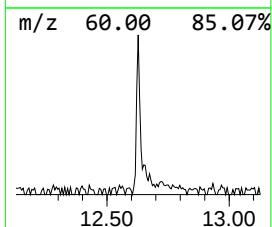
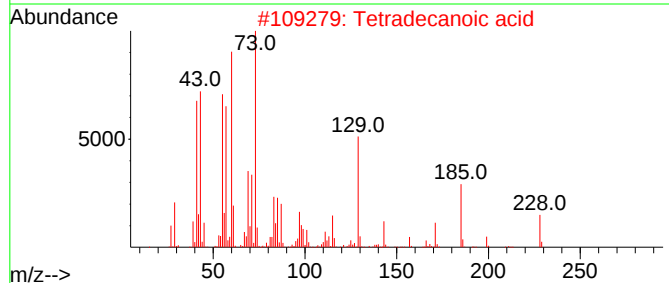
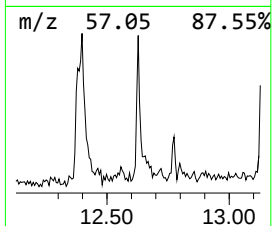
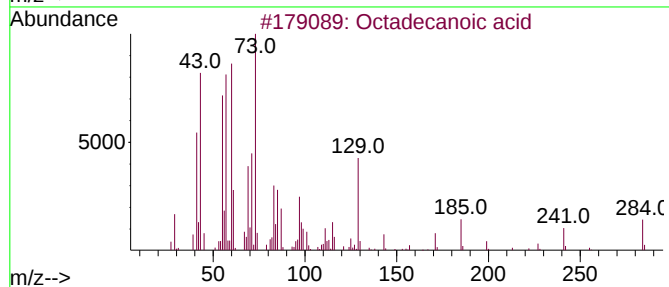
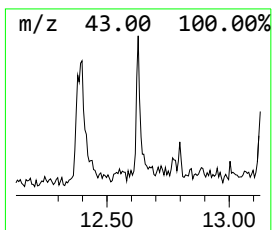
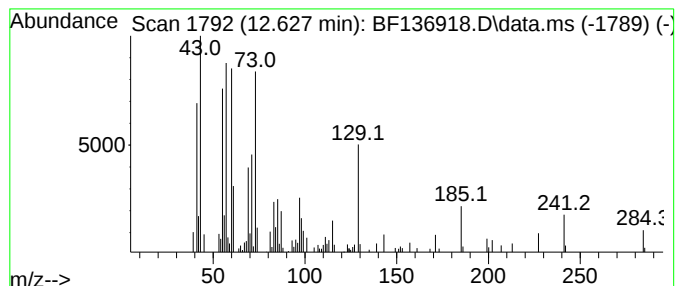
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	3.55 ng	89769	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3			Undecanoic acid	186	C11H22O2	000112-37-8	60
4			n-Decanoic acid	172	C10H20O2	000334-48-5	52
5			Xylose	150	C5H10O5	000058-86-6	22



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-21

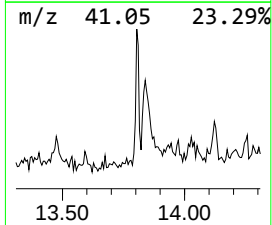
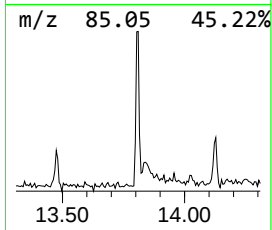
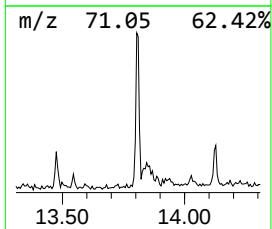
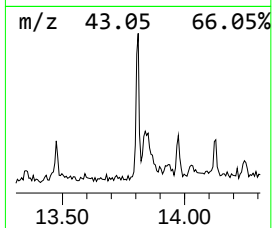
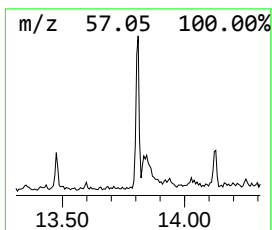
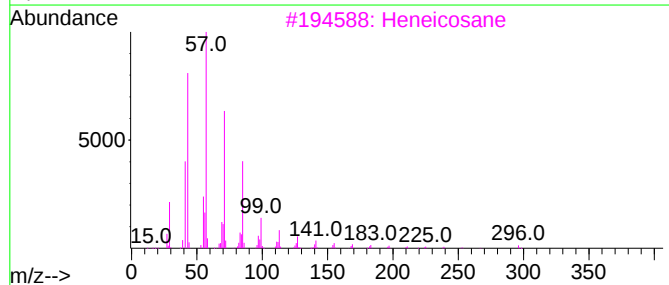
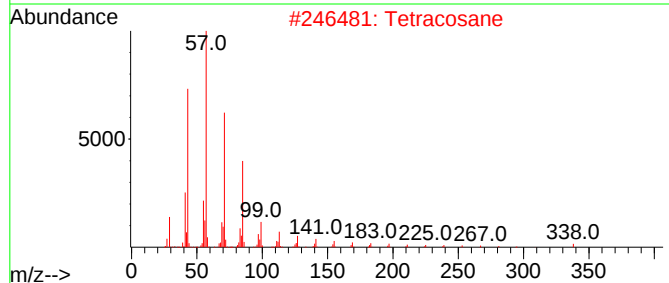
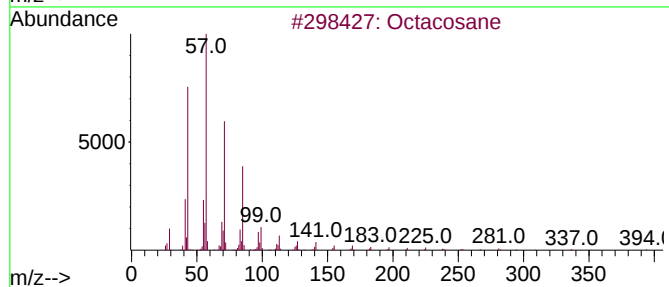
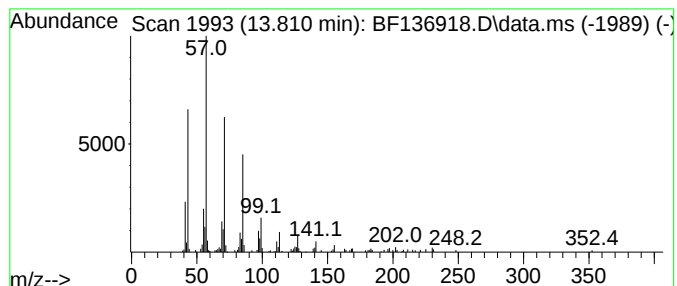
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	4.16 ng	85325	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91



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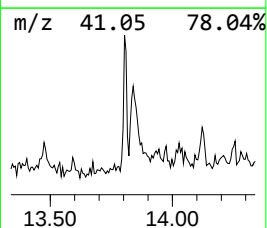
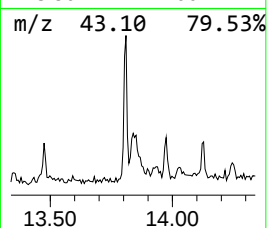
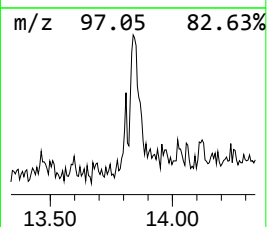
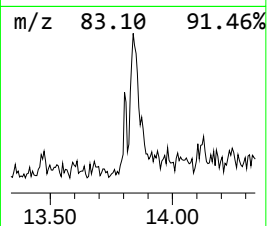
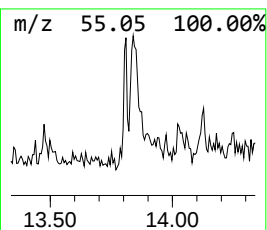
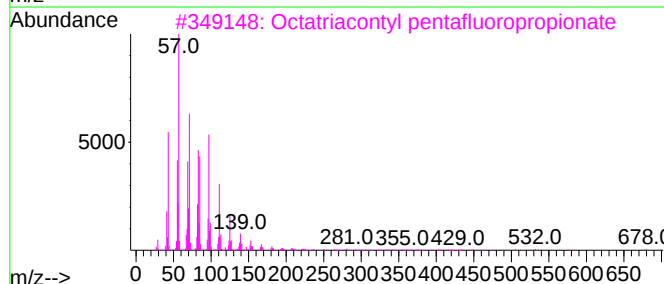
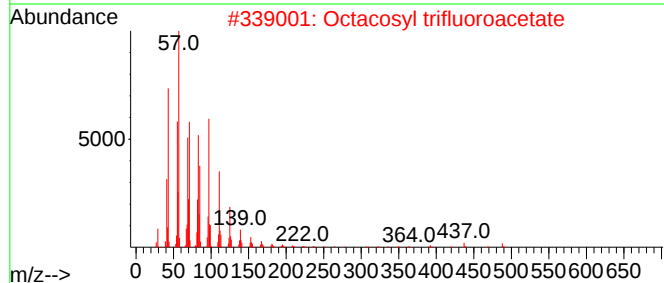
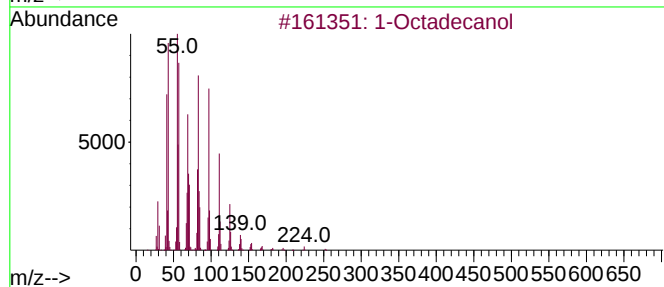
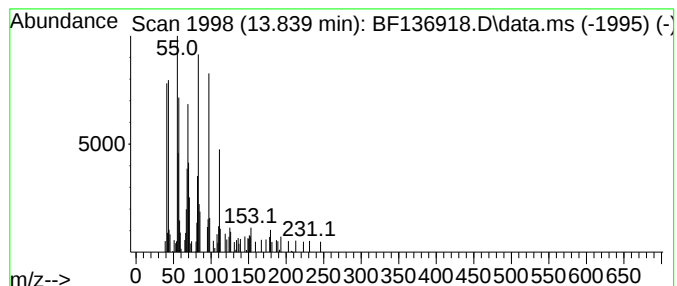
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Octadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	5.04 ng	103329	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanol	270	C18H38O	000112-92-5	87
2			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	83
3			Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	80
4			Cyclohexadecane	224	C16H32	000295-65-8	62
5			1-Hexadecanol	242	C16H34O	036653-82-4	58



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Acq On : 03 Jan 2024 20:51
Operator : CG\JU
Sample : 05897-17
Misc :
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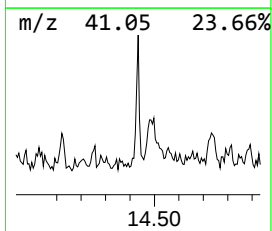
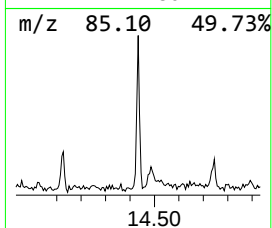
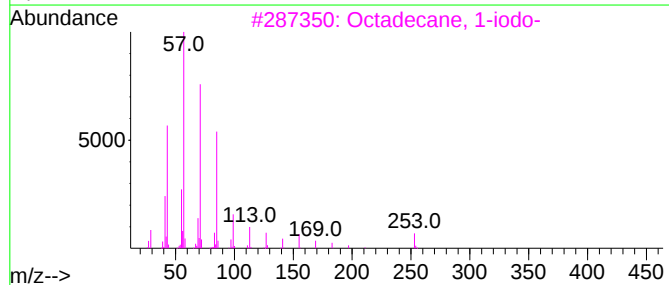
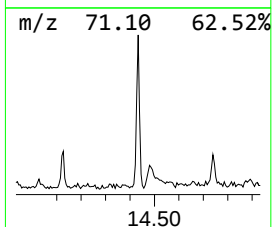
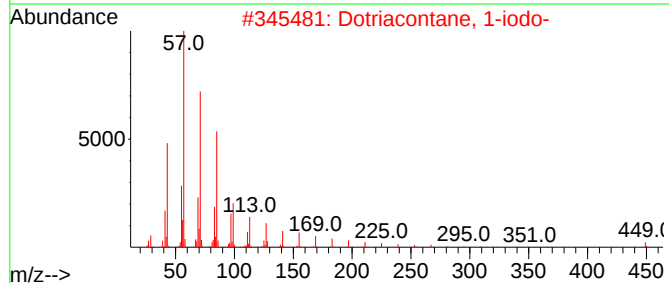
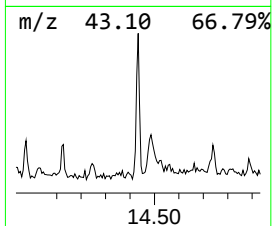
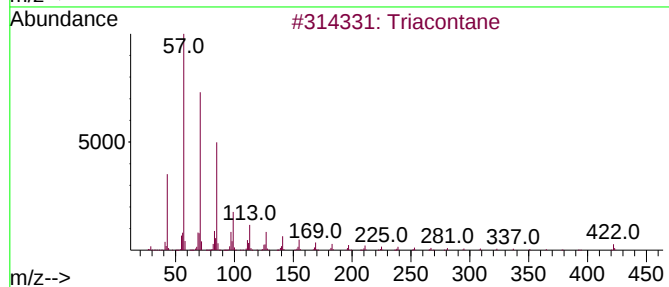
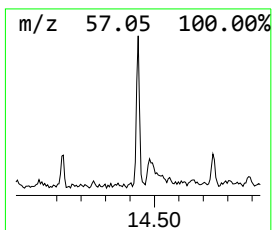
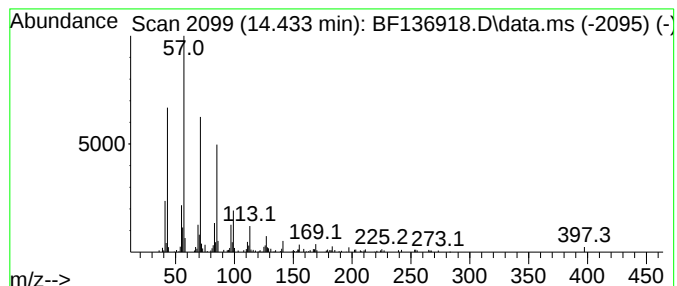
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.433	5.18 ng	106210	Chrysene-d12		13.963	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Triacontane		422	C30H62	000638-68-6	91
2	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	91
3	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	90
4	Eicosane, 1-iodo-		408	C20H41I	1000406-31-8	90
5	Docosane, 1-iodo-		436	C22H45I	1000406-31-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
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Sample : 05897-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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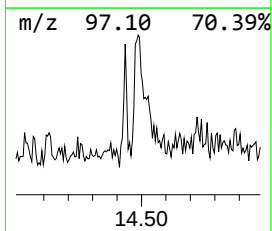
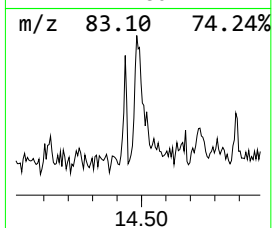
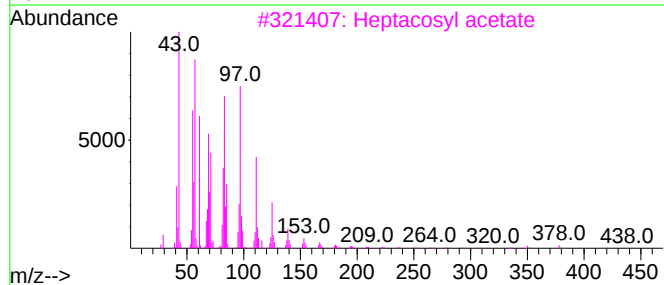
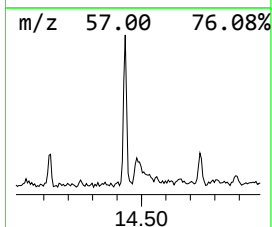
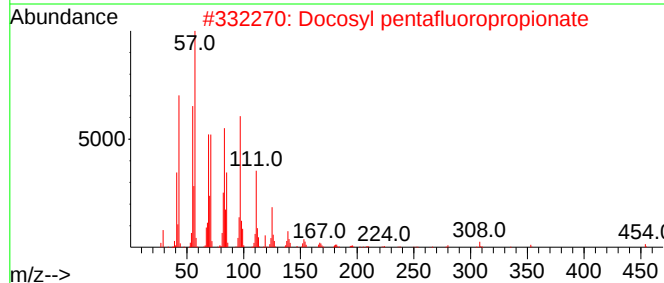
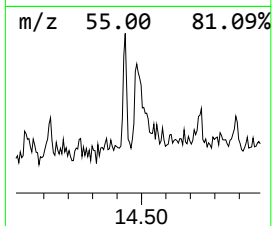
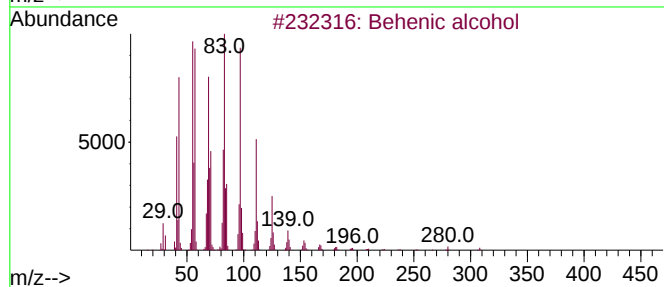
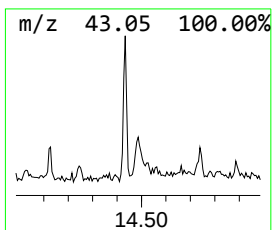
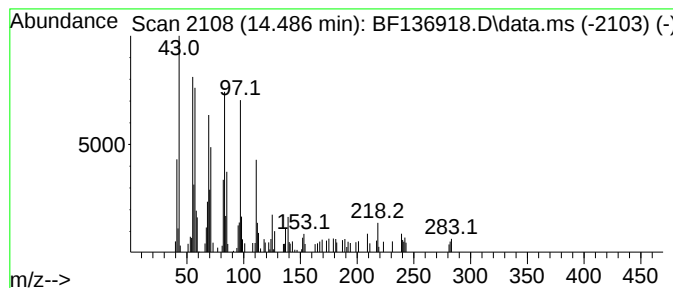
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	3.89 ng	79844	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	93
2			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
3			Heptacosyl acetate	438	C29H58O2	1000351-78-2	83
4			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	83
5			Dotriacontyl propyl ether	509	C35H72O	1000406-28-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136918.D
Acq On : 03 Jan 2024 20:51
Operator : CG\JU
Sample : 05897-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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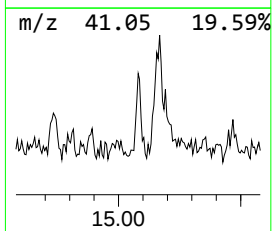
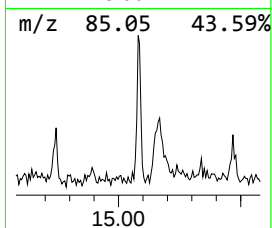
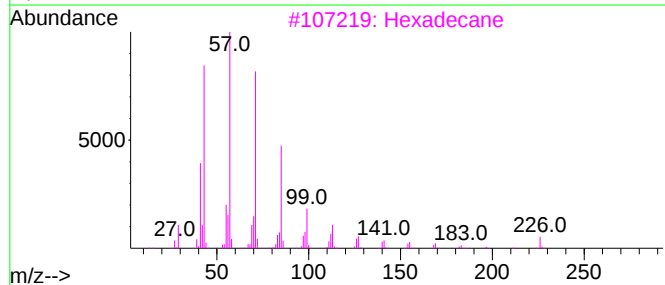
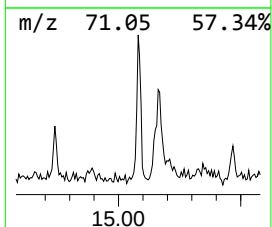
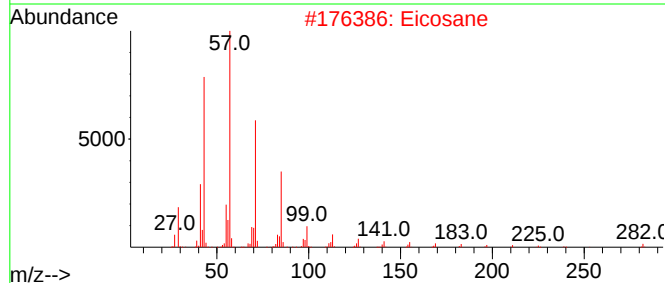
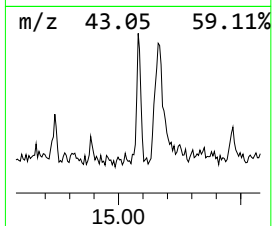
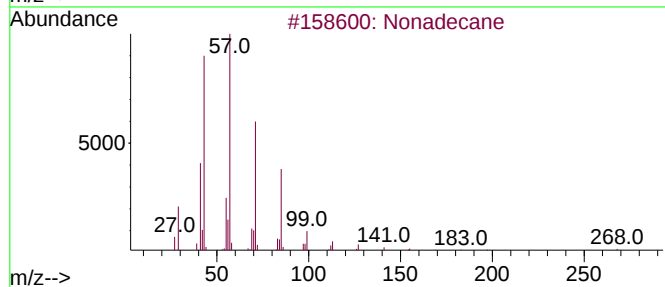
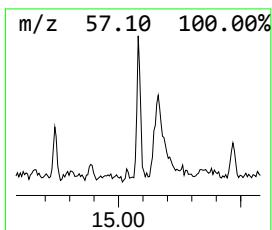
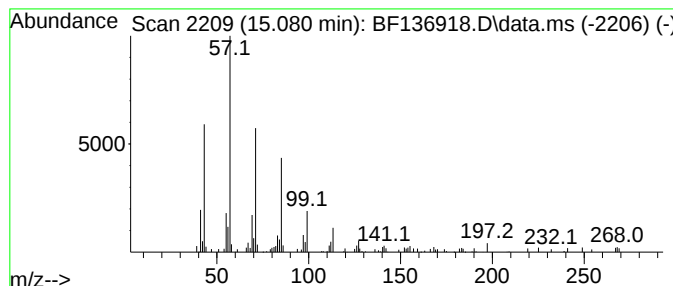
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	3.31 ng	69162	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	89
2			Eicosane	282	C20H42	000112-95-8	80
3			Hexadecane	226	C16H34	000544-76-3	72
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
5			Heptadecane	240	C17H36	000629-78-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136918.D
Acq On : 03 Jan 2024 20:51
Operator : CG\JU
Sample : 05897-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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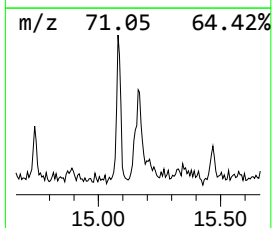
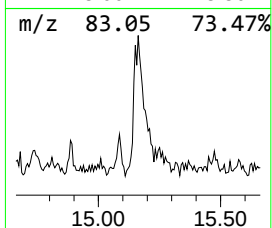
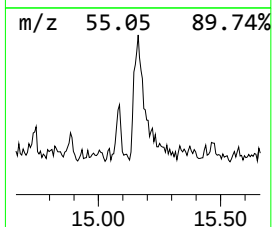
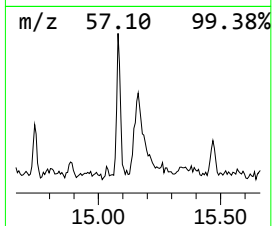
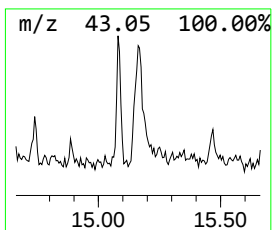
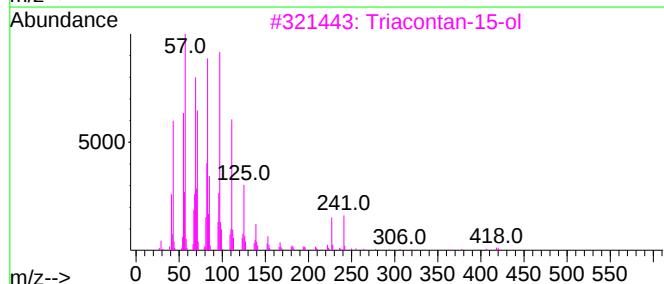
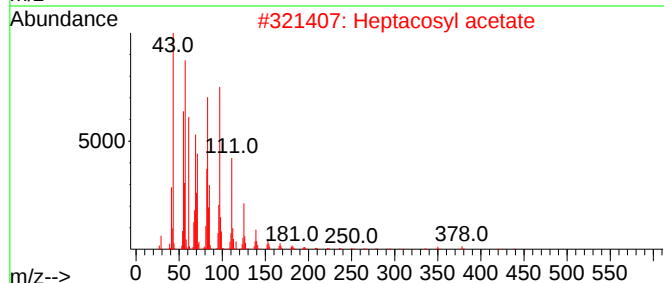
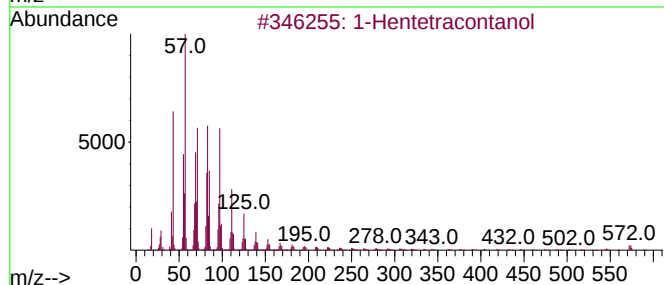
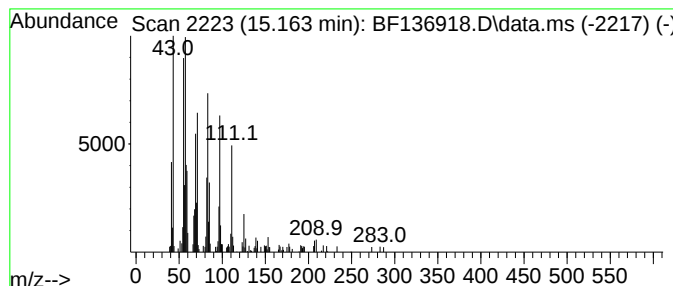
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Hentetracontanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	10.07 ng	210397	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hentetracontanol	593	C41H84O	040710-42-7	68
2			Heptacosyl acetate	438	C29H58O2	1000351-78-2	64
3			Triacontan-15-ol	438	C30H62O	031849-26-0	64
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	64
5			Octacosanol	410	C28H58O	000557-61-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
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Operator : CG\JU
Sample : 05897-17
Misc :
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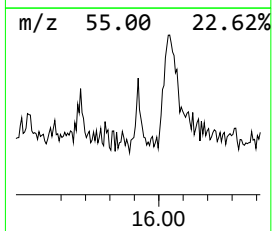
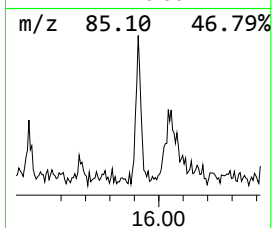
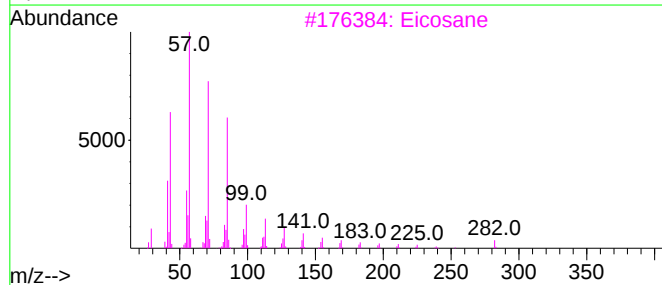
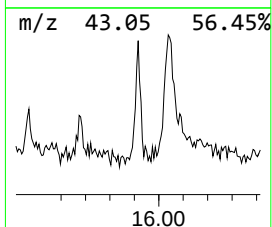
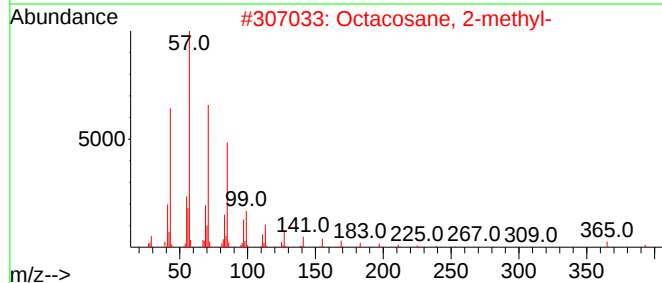
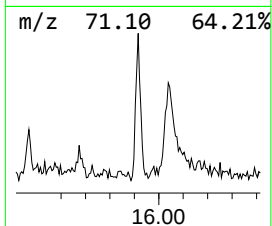
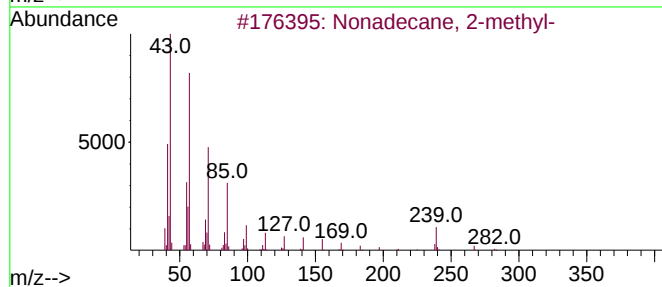
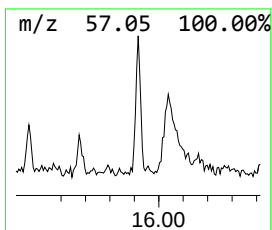
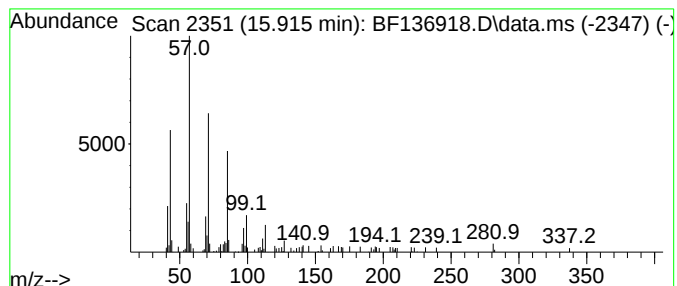
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.915	2.74 ng	57298	Perylene-d12	15.445	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3	Eicosane	282	C20H42	000112-95-8	86
4	Hexacosane	366	C26H54	000630-01-3	86
5	Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136918.D
Acq On : 03 Jan 2024 20:51
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Sample : 05897-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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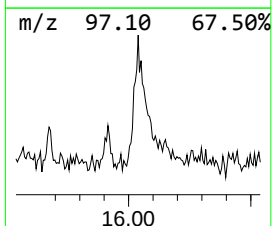
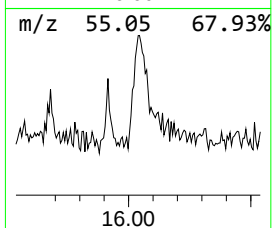
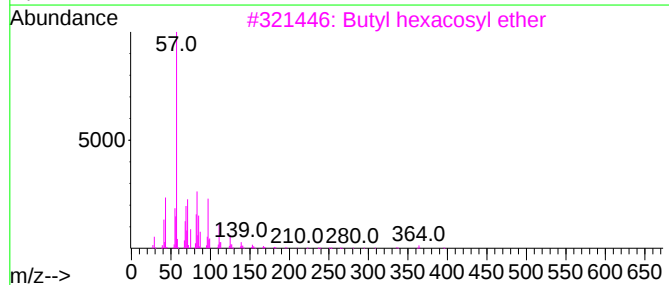
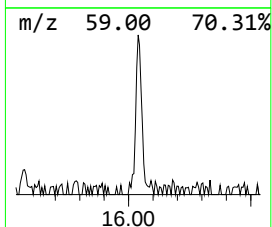
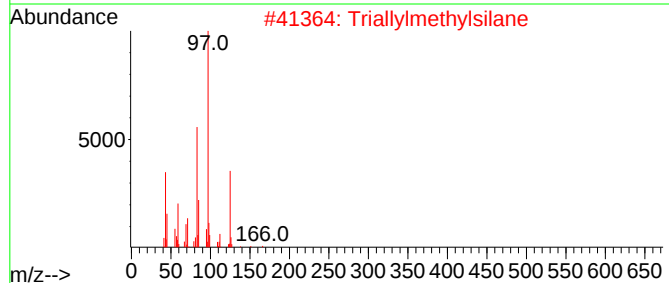
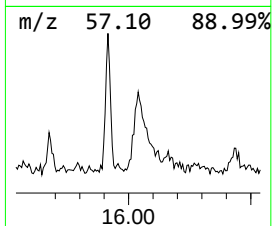
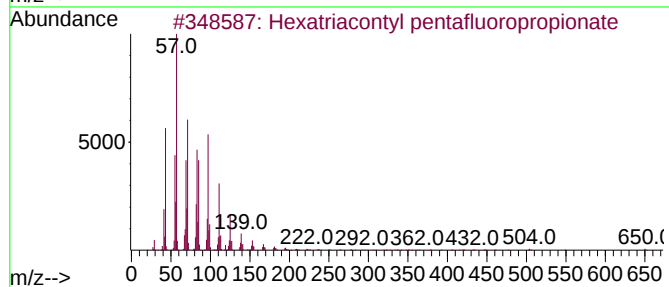
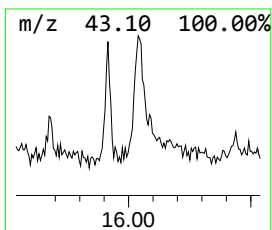
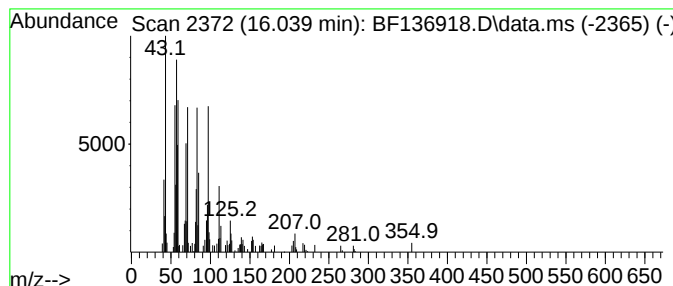
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexatriacontyl pentafluorop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	10.31 ng	215299	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	53
2			Triallylmethylsilane	166	C10H18Si	001112-91-0	53
3			Butyl hexacosyl ether	438	C30H62O	1000406-41-0	53
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	53
5			Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136918.D
Acq On : 03 Jan 2024 20:51
Operator : CG\JU
Sample : 05897-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
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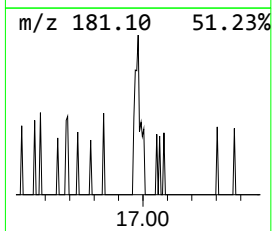
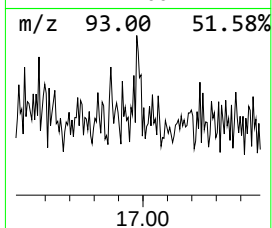
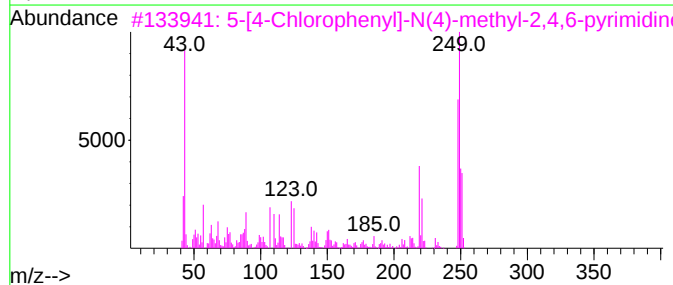
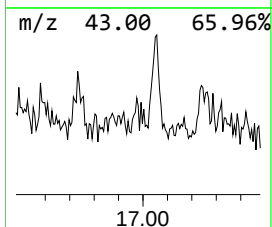
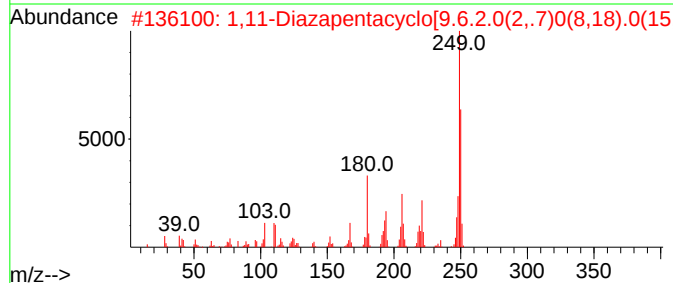
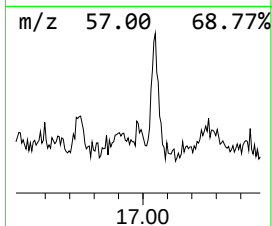
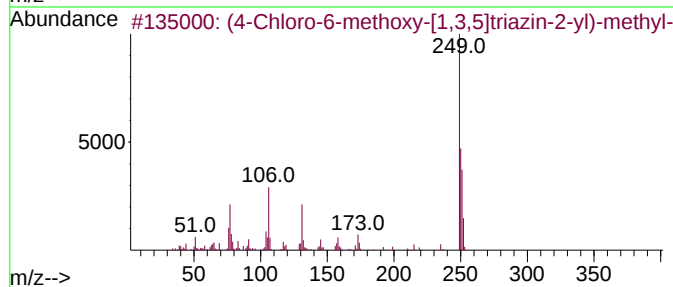
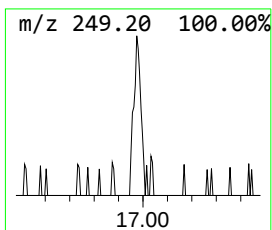
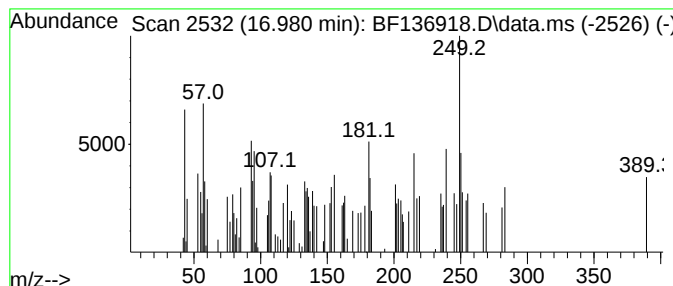
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.980 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.980	2.10 ng	43883	Perylene-d12	15.445

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(4-Chloro-6-methoxy-[1,3,5]triaz...	250	C11H11ClN4O	059881-58-2	35
2		1,11-Diazapentacyclo[9.6.2.0(2,...	250	C17H18N2	1000436-58-8	35
3		5-[4-Chlorophenyl]-N(4)-methyl-2...	249	C11H12ClN5	1000212-53-8	27
4		Phosphine, methyl-(2,4,6-triisop...	250	C16H27P	158748-69-7	27
5		1-Chloro-3-nitro-5-phenoxybenzene	249	C12H8ClNO3	1000444-79-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136918.D
Acq On : 03 Jan 2024 20:51
Operator : CG\JU
Sample : 05897-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-21

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.839	9.8	ng	248747	4	11.304	506003	20.0
1-Tricosene	12.392	5.6	ng	142644	4	11.304	506003	20.0
Octadecanoic acid	12.627	3.5	ng	89769	4	11.304	506003	20.0
Octacosane	13.810	4.2	ng	85325	5	13.963	409984	20.0
1-Octadecanol	13.839	5.0	ng	103329	5	13.963	409984	20.0
Triacontane	14.433	5.2	ng	106210	5	13.963	409984	20.0
Behenic alcohol	14.486	3.9	ng	79844	5	13.963	409984	20.0
Nonadecane	15.080	3.3	ng	69162	6	15.445	417762	20.0
1-Hentetracontanol	15.163	10.1	ng	210397	6	15.445	417762	20.0
Nonadecane, 2-m...	15.915	2.7	ng	57298	6	15.445	417762	20.0
Hexatriacontyl ...	16.039	10.3	ng	215299	6	15.445	417762	20.0
unknown16.980	16.980	2.1	ng	43883	6	15.445	417762	20.0