

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

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-BF122921.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126503.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.993	490	494	502	rVB	48269	59561	2.36%	0.318%
2	5.399	558	563	566	rBV	2516198	2314772	91.69%	12.364%
3	6.416	730	736	739	rBV	2443261	2436271	96.51%	13.013%
4	6.781	794	798	801	rBV	747169	583375	23.11%	3.116%
5	7.345	888	894	897	rBV	1620291	1625118	64.38%	8.680%
6	8.063	1012	1016	1019	rBV	973313	814149	32.25%	4.349%
7	9.145	1194	1200	1203	rBV	2520857	2524428	100.00%	13.484%
8	9.228	1210	1214	1218	rVB	45531	37521	1.49%	0.200%
9	9.628	1280	1282	1289	rVB2	21057	26068	1.03%	0.139%
10	9.816	1310	1314	1318	rBV	948046	862213	34.15%	4.605%
11	10.610	1444	1449	1452	rBV	1558982	1470136	58.24%	7.853%
12	11.304	1563	1567	1570	rBV	1019899	831147	32.92%	4.439%
13	11.704	1631	1635	1638	rVB	35605	28928	1.15%	0.155%
14	11.839	1654	1658	1662	rBV	264730	229411	9.09%	1.225%
15	12.622	1788	1791	1797	rBV	109982	132935	5.27%	0.710%
16	12.716	1805	1807	1812	rVB2	41562	32945	1.31%	0.176%
17	12.892	1833	1837	1841	rBV	2344408	2360867	93.52%	12.610%
18	13.374	1911	1919	1923	rBV4	18913	27794	1.10%	0.148%
19	13.451	1923	1932	1934	rBV2	30937	40092	1.59%	0.214%
20	13.798	1985	1991	1999	rBV2	119469	202467	8.02%	1.081%
21	13.939	2011	2015	2019	rBV	719631	657113	26.03%	3.510%
22	14.039	2027	2032	2039	rBV	137441	143885	5.70%	0.769%
23	14.116	2041	2045	2051	rBV	23745	26900	1.07%	0.144%
24	14.421	2093	2097	2103	rBV	25292	34450	1.36%	0.184%
25	14.698	2140	2144	2152	rBV	408146	471433	18.67%	2.518%
26	14.798	2157	2161	2165	rVB	57000	60992	2.42%	0.326%
27	15.051	2201	2204	2210	rVB2	28812	28801	1.14%	0.154%
28	15.380	2255	2260	2264	rBV	449358	519589	20.58%	2.775%
29	15.421	2264	2267	2271	rVB	29694	35916	1.42%	0.192%
30	15.839	2334	2338	2344	rVB2	27867	37288	1.48%	0.199%
31	16.333	2416	2422	2427	rBV3	22168	37444	1.48%	0.200%
32	16.904	2514	2519	2524	rVB4	14127	27664	1.10%	0.148%

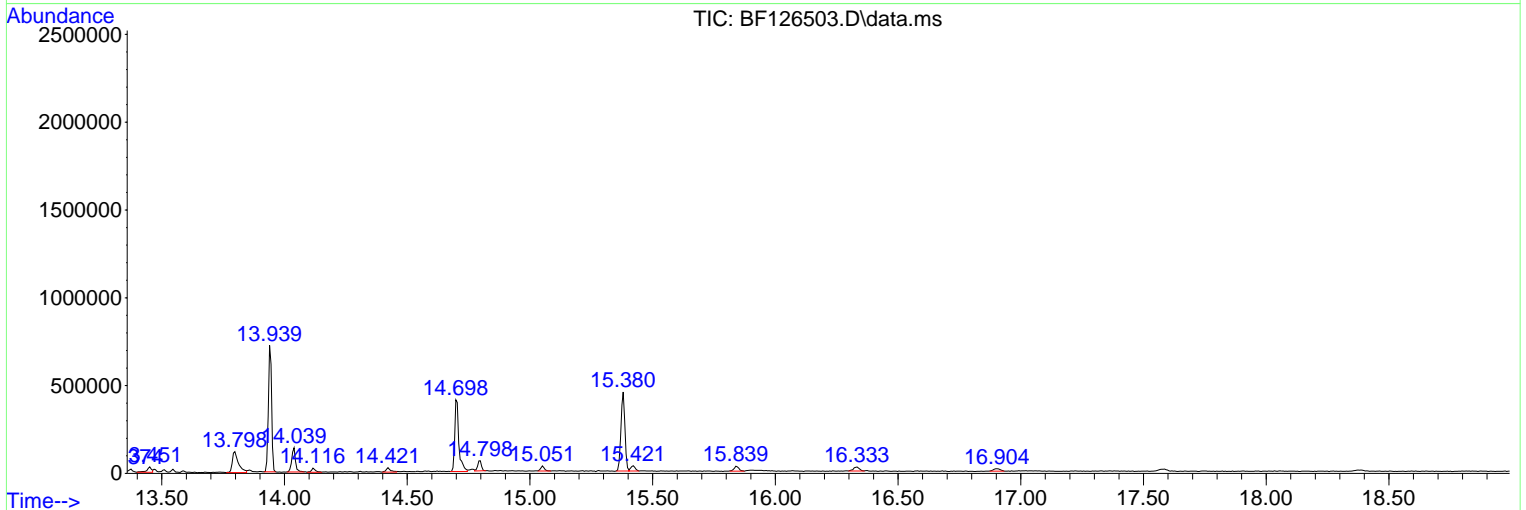
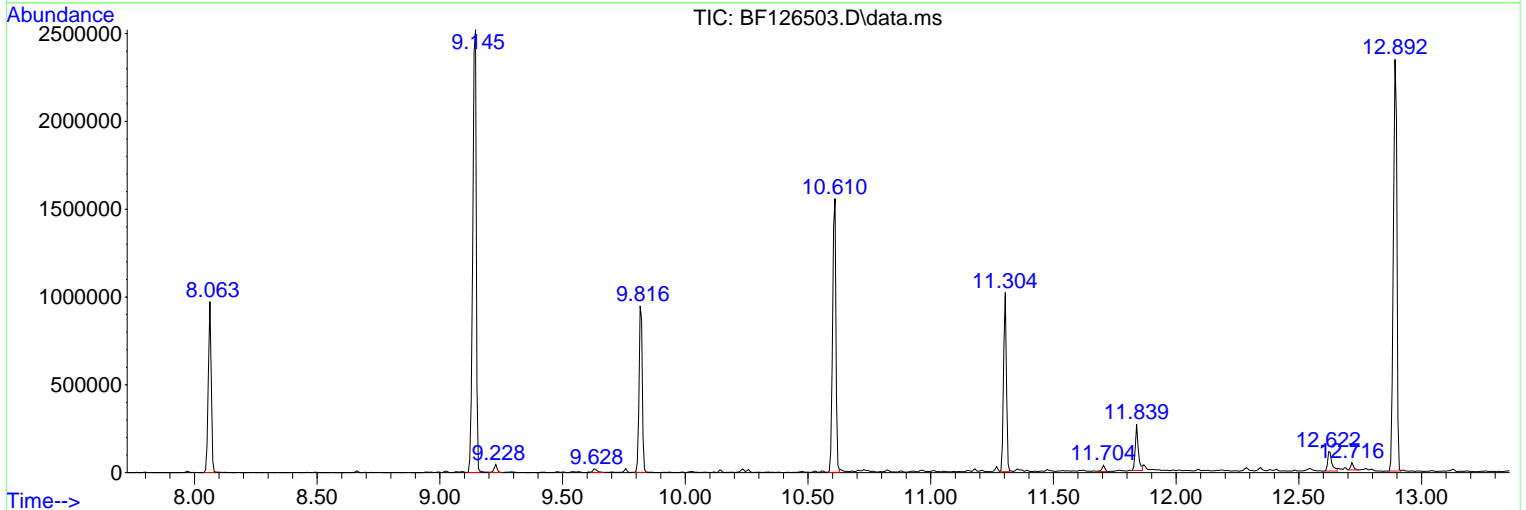
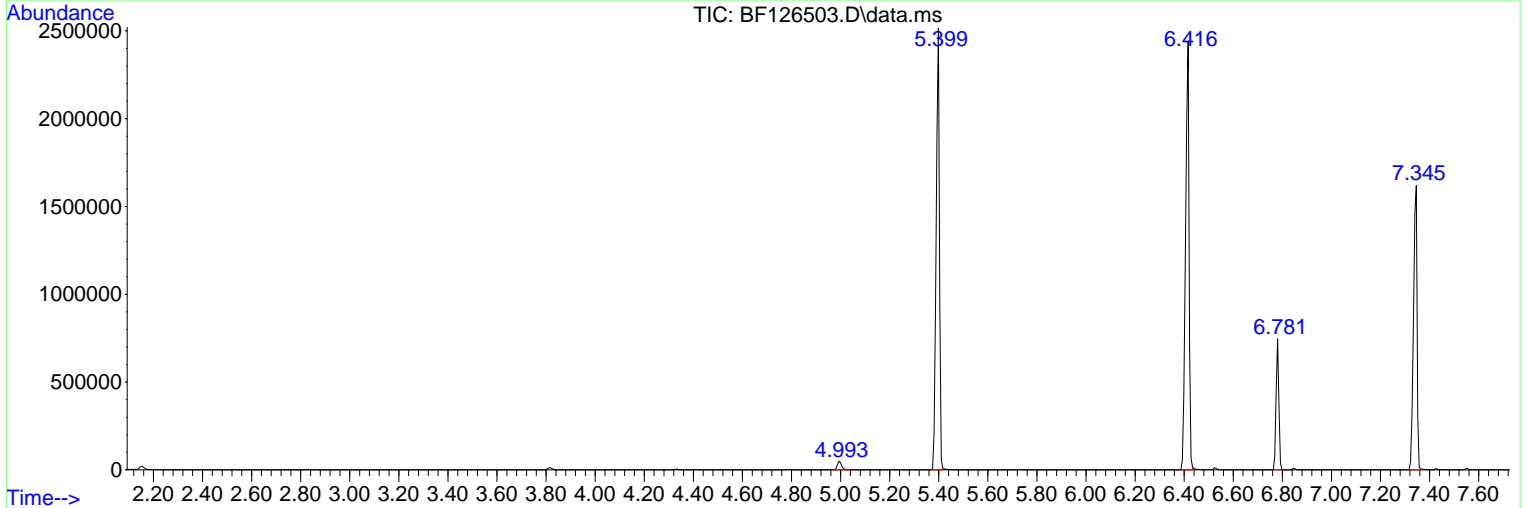
Sum of corrected areas: 18721673

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

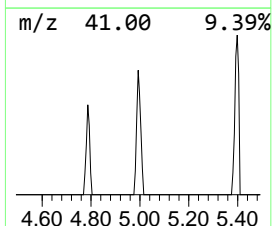
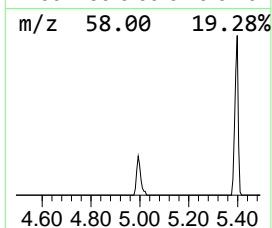
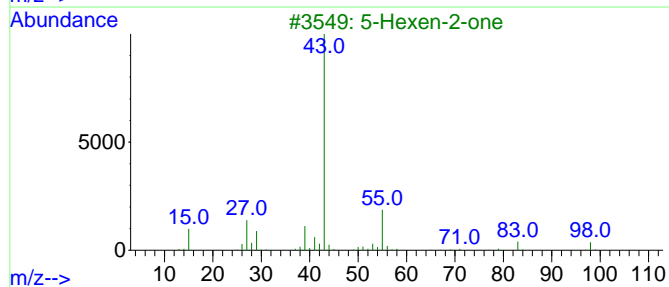
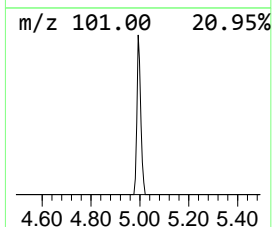
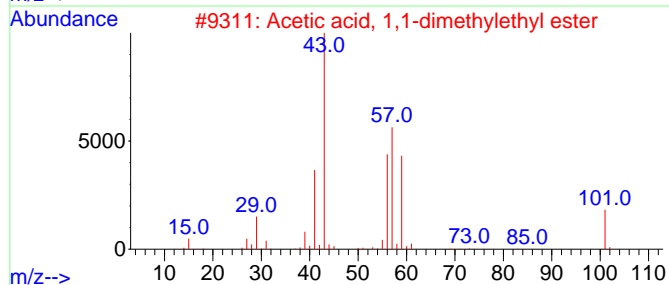
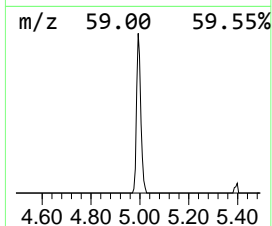
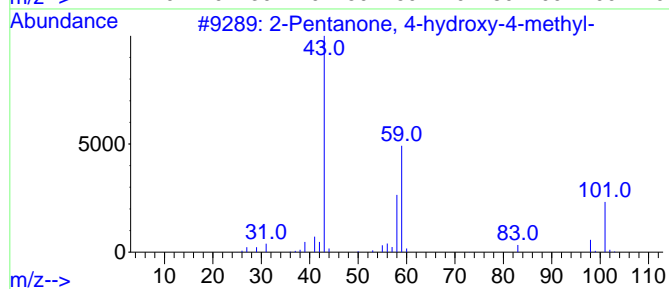
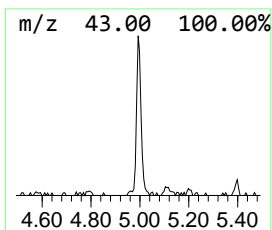
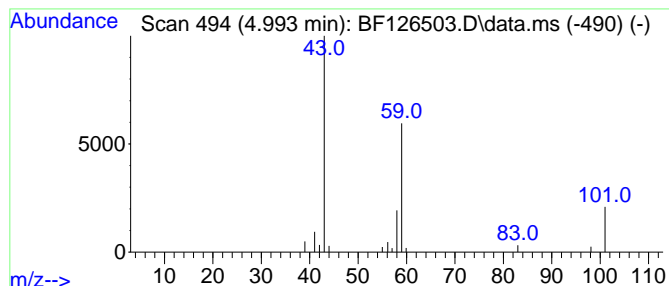
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.993	2.04 ng	59561	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

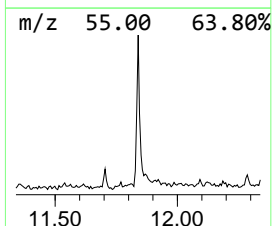
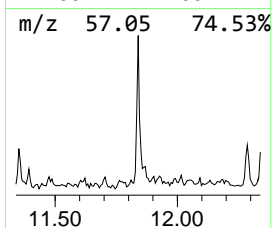
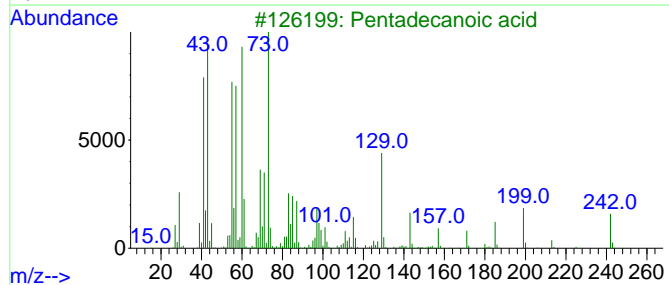
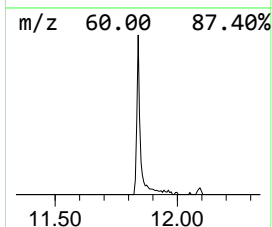
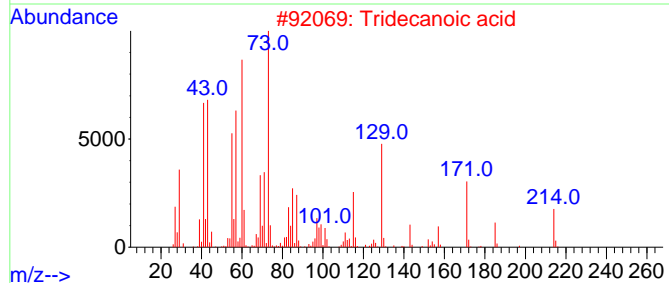
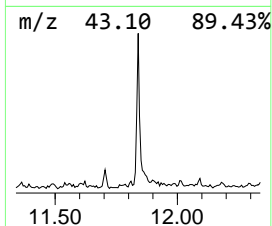
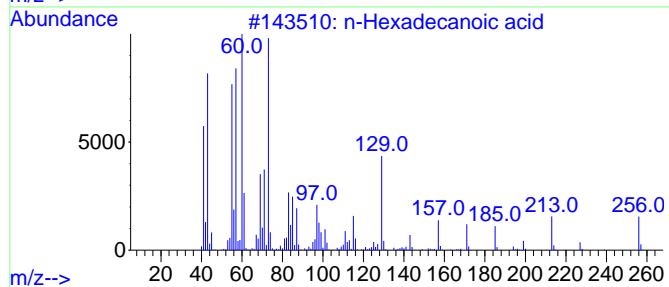
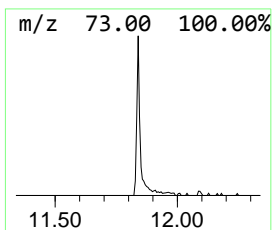
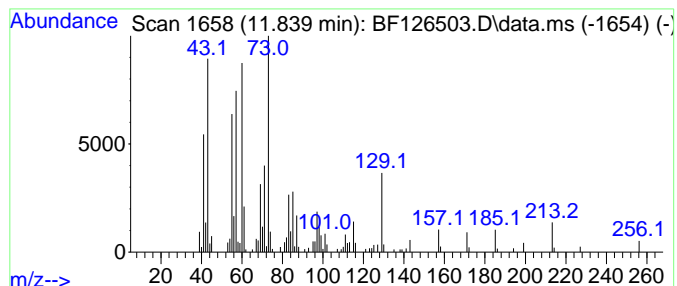
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.839	5.52 ng	229411	Phenanthrene-d10	11.304

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Nonanoic acid	158	C9H18O2	000112-05-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

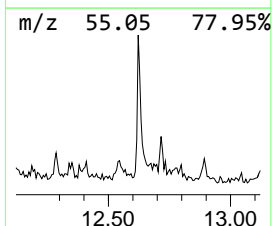
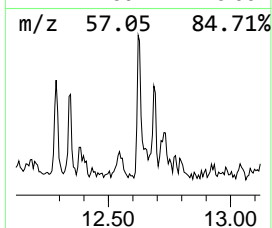
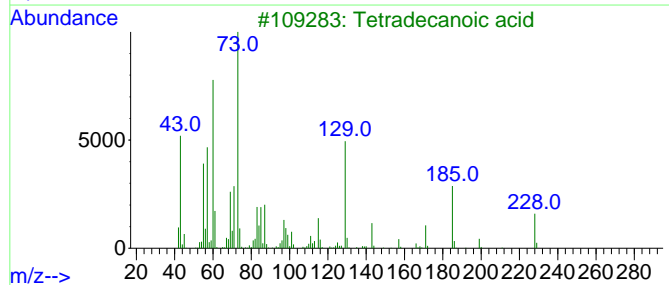
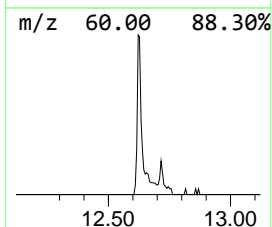
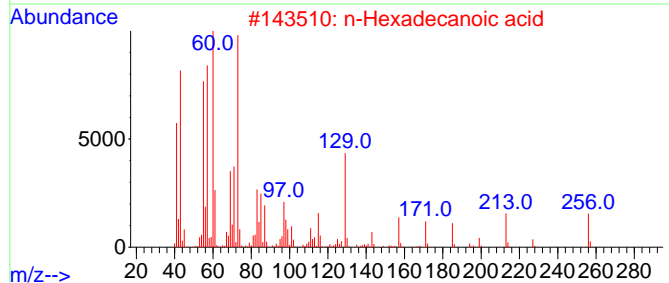
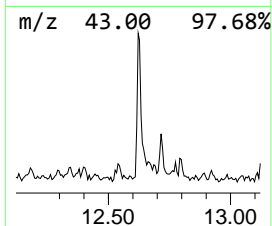
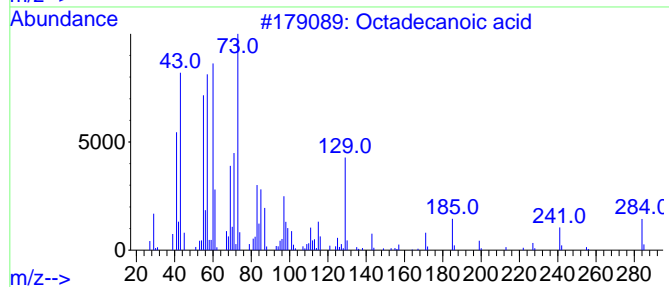
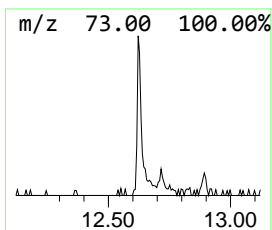
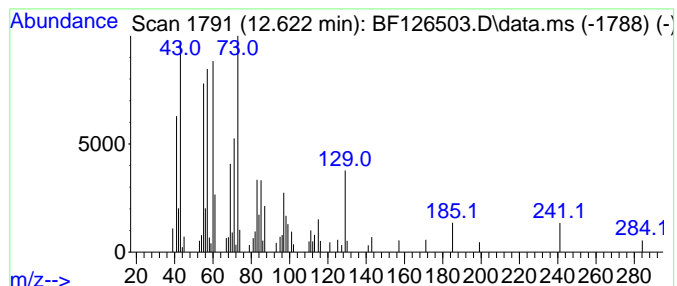
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.622	3.20 ng	132935	Phenanthrene-d10	11.304

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25
5		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

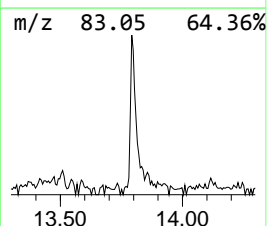
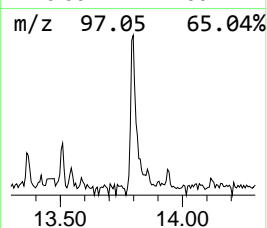
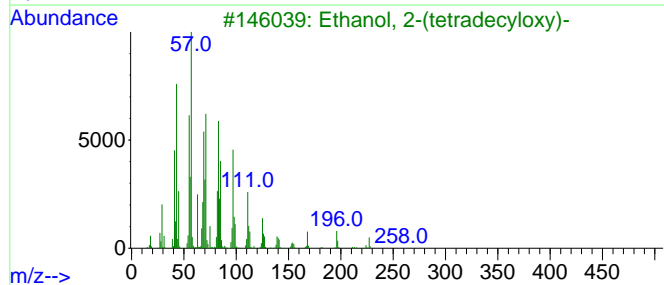
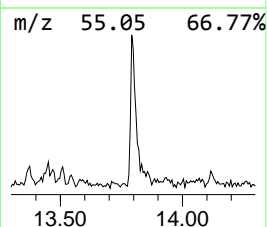
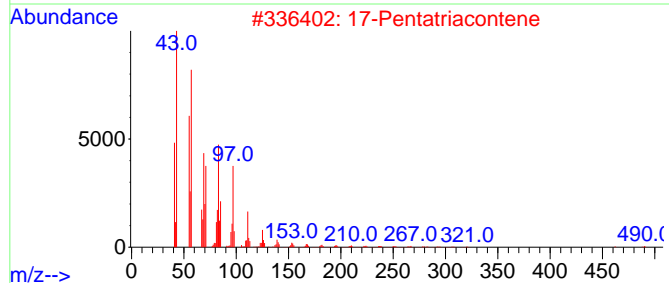
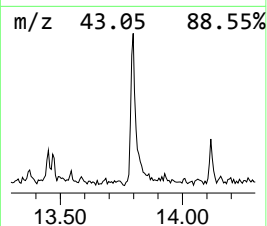
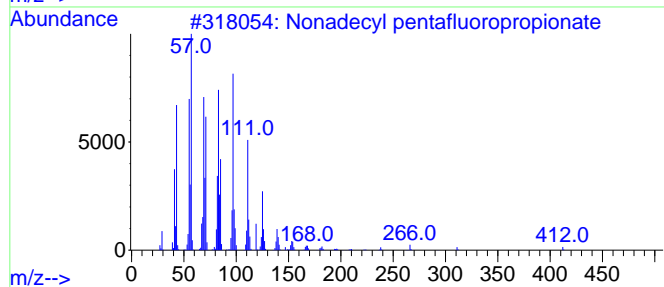
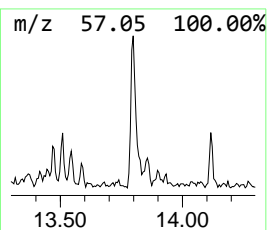
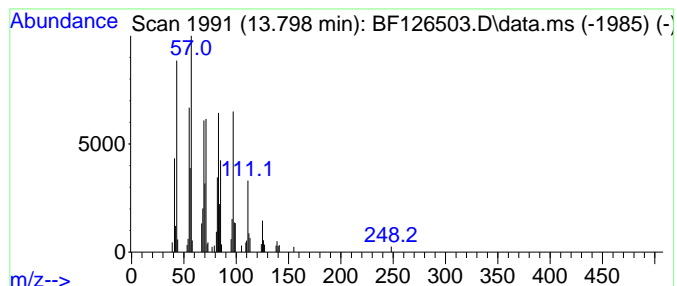
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 4 Nonadecyl pentafluoropropio... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	6.16 ng	202467	Chrysene-d12	13.939

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4		1-Hexacosene	364	C26H52	018835-33-1	87
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

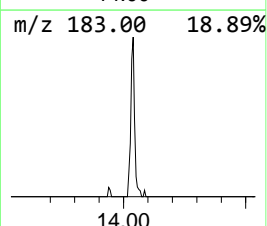
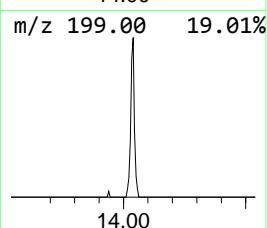
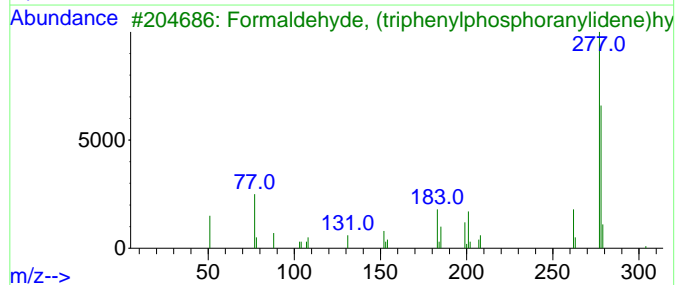
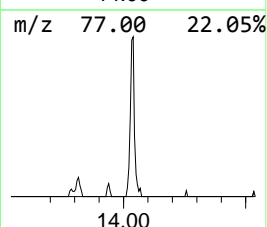
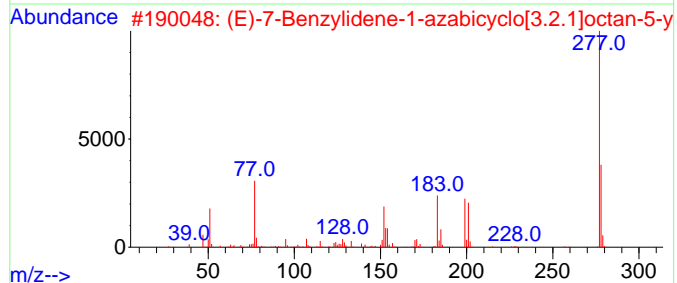
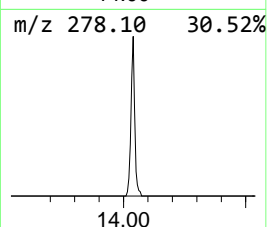
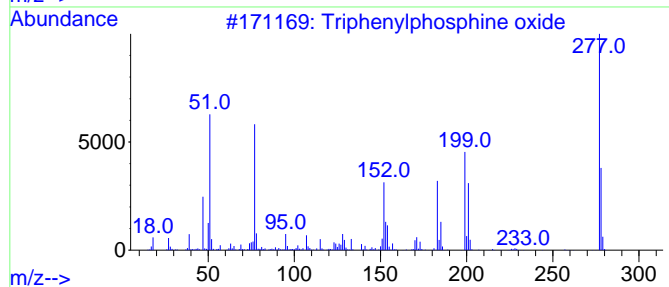
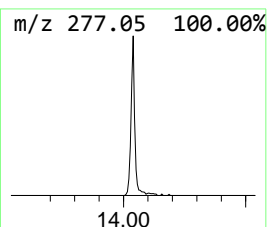
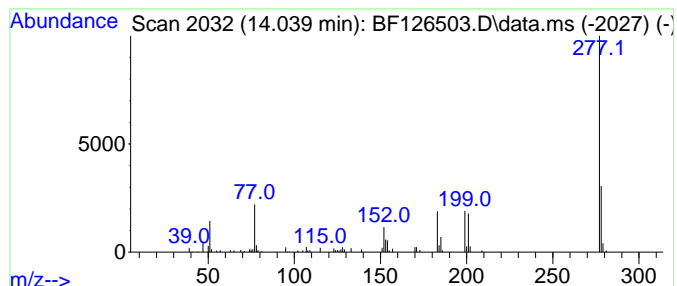
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.039	4.38 ng	143885	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Vanadium, cycloheptatrieny1-(pen...	277	C17H22V	1000155-20-5	50
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

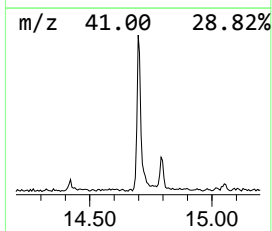
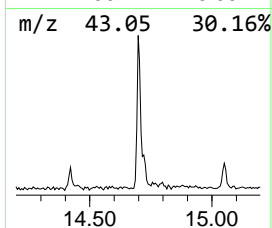
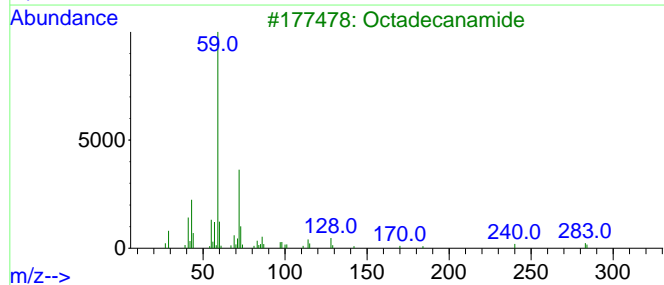
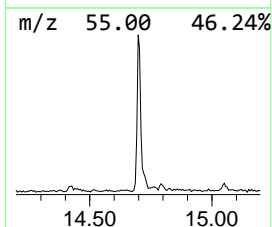
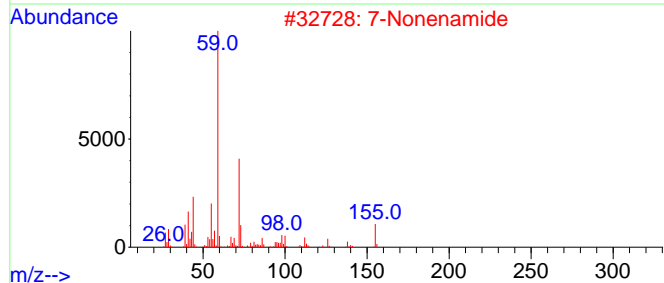
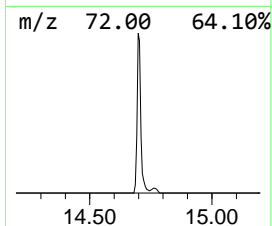
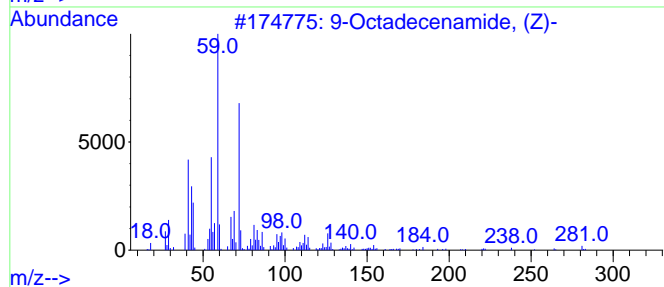
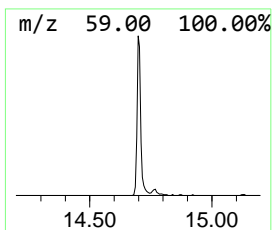
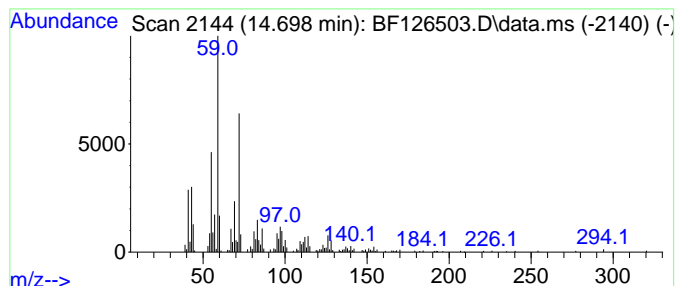
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.698	18.15 ng	471433	Perylene-d12	15.380

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		7-Nonenamide	155	C9H17NO	090949-53-4	72
3		Octadecanamide	283	C18H37NO	000124-26-5	59
4		Hexadecanamide	255	C16H33NO	000629-54-9	59
5		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

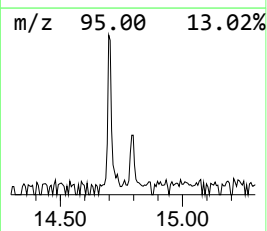
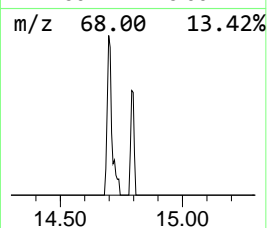
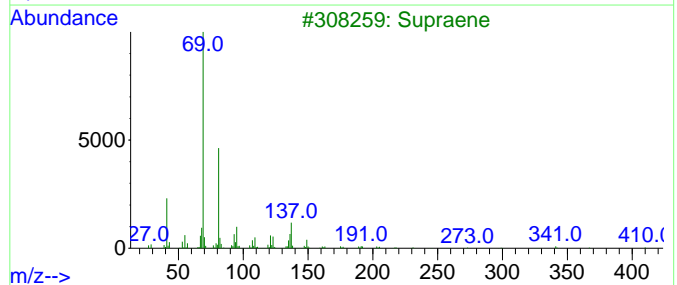
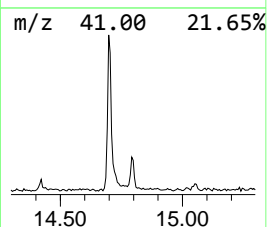
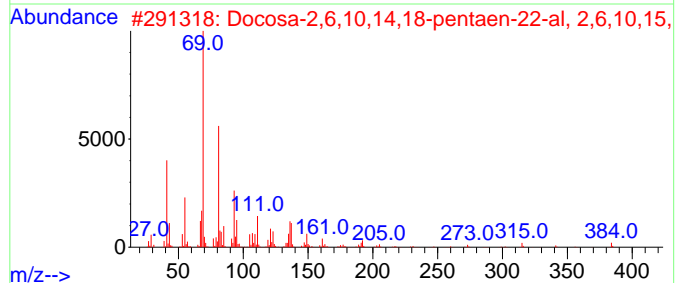
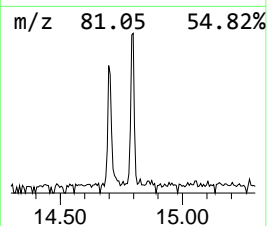
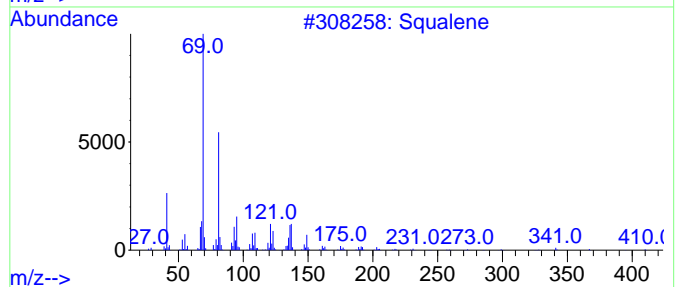
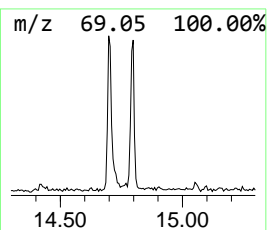
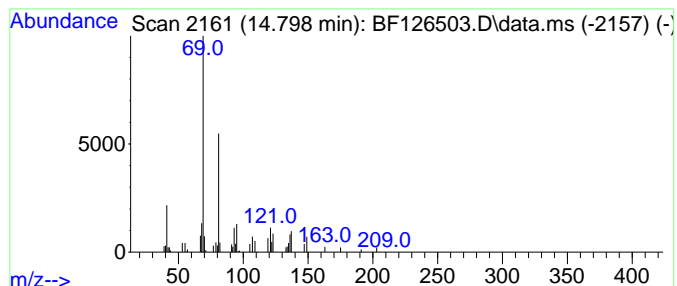
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	2.35 ng	60992	Perylene-d12	15.380

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	87
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
3			Supraene	410	C30H50	007683-64-9	86
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
5			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010522\
 Data File : BF126503.D
 Acq On : 5 Jan 2022 18:40
 Operator : JU/CG
 Sample : M5196-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-SAMPLE-2-DEEP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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-...	4.993	2.0	ng	59561	1	6.781	583375	20.0
n-Hexadecanoic ...	11.839	5.5	ng	229411	4	11.304	831147	20.0
Octadecanoic acid	12.622	3.2	ng	132935	4	11.304	831147	20.0
Nonadecyl penta...	13.798	6.2	ng	202467	5	13.939	657113	20.0
Triphenylphosph...	14.039	4.4	ng	143885	5	13.939	657113	20.0
9-Octadecenamid...	14.698	18.1	ng	471433	6	15.380	519589	20.0
Squalene	14.798	2.4	ng	60992	6	15.380	519589	20.0