LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134349.D
Acq On : 18 Jul 2023 21:23
Operator : CG\JU
Sample : 03597-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134349.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.081	506	509	521	rVB	20952	28241	1.65%	0.217%
2	5.475	572	576	593	rBV	1459772	1345128	78.71%	10.315%
3	6.481	742	747	750	rBV	1478558	1335974	78.18%	10.245%
4	6.839	804	808	811	rBV	461212	389874	22.81%	2.990%
5	7.404	899	904	914	rBV	901056	892716	52.24%	6.846%
6	8.116	1021	1025	1040	rBV	643595	512542	29.99%	3.931%
7	9.192	1204	1208	1211	rBV	2252147	1708896	100.00%	13.105%
8	9.875	1320	1324	1327	rBV	627928	531115	31.08%	4.073%
9	10.669	1455	1459	1474	rBV	1205275	1052434	61.59%	8.071%
10	11.369	1574	1578	1581	rBV	592498	487465	28.53%	3.738%
11	11.898	1664	1668	1676	rBV	124249	134482	7.87%	1.031%
12	12.780	1815	1818	1822	rBV	142778	115620	6.77%	0.887%
13	12.963	1845	1849	1853	rBV	1565433	1386221	81.12%	10.631%
14	13.451	1923	1932	1933	rBV	607950	644215	37.70%	4.940%
15	13.463	1933	1934	1941	rVV	695356	494299	28.93%	3.791%
16	13.521	1941	1944	1949	rVB	103495	93785	5.49%	0.719%
17	13.898	2000	2008	2021	rBV4	60253	163124	9.55%	1.251%
18	14.027	2027	2030	2034	rBV	422763	386813	22.64%	2.966%
19	14.121	2041	2046	2050	rBV	295280	306157	17.92%	2.348%
20	14.315	2075	2079	2082	rBV4	24971	28851	1.69%	0.221%
21	14.545	2114	2118	2121	rBV5	14206	24479	1.43%	0.188%
22	14.798	2156	2161	2170	rBV	338610	555869	32.53%	4.263%
23	15.533	2282	2286	2293	rBV	308326	393472	23.02%	3.017%
24	16.009	2363	2367	2371	rBV2	18137	28124	1.65%	0.216%

Sum of corrected areas: 13039896

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
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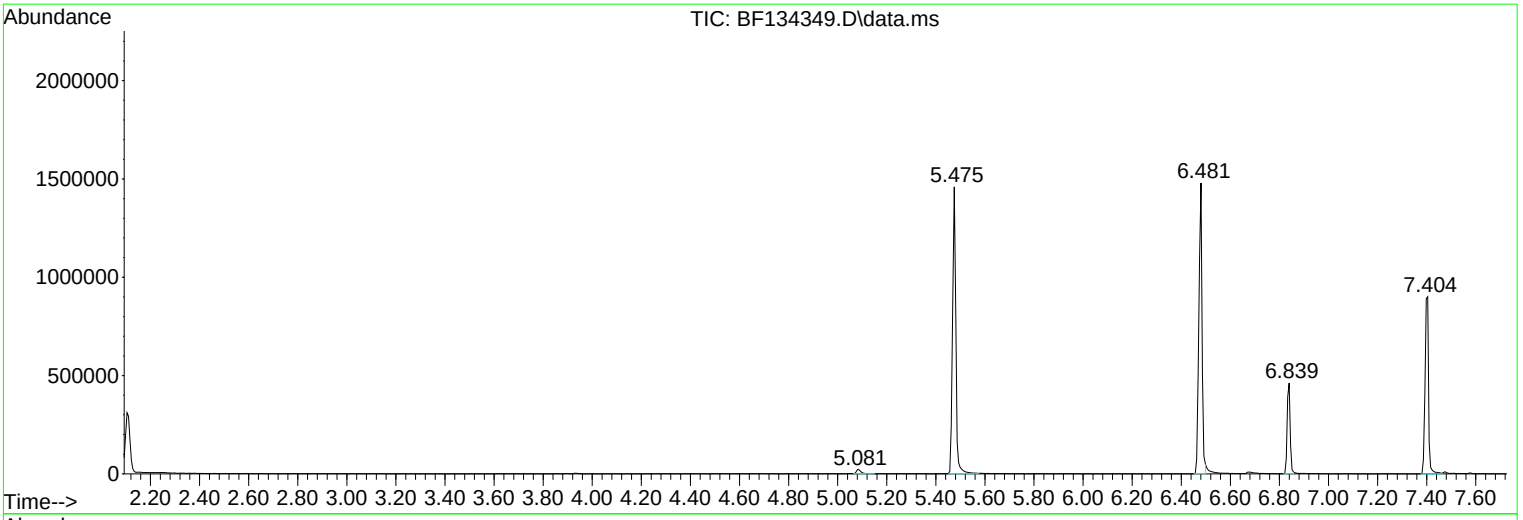
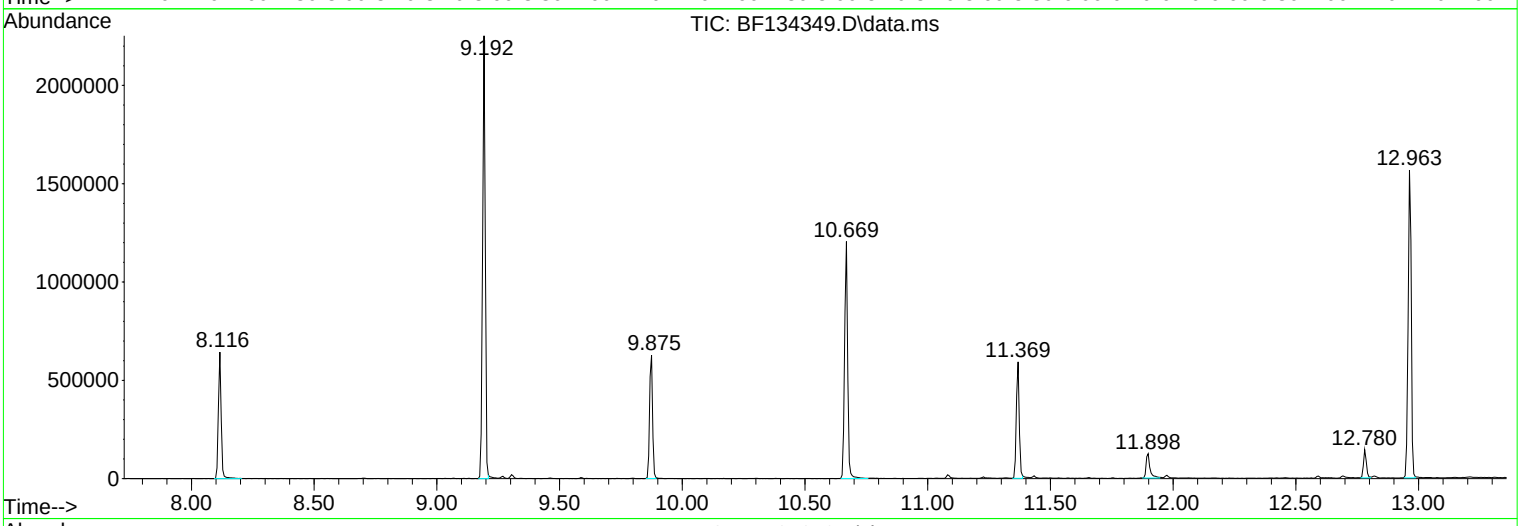
Operator : CG\JU
Sample : 03597-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

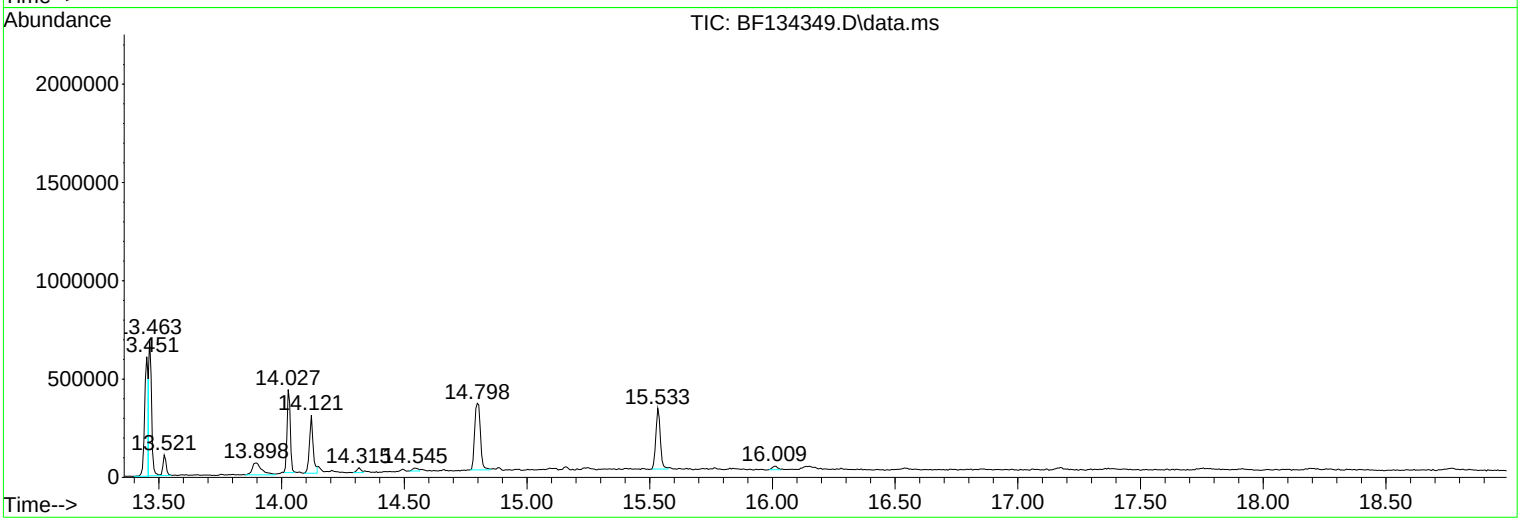
Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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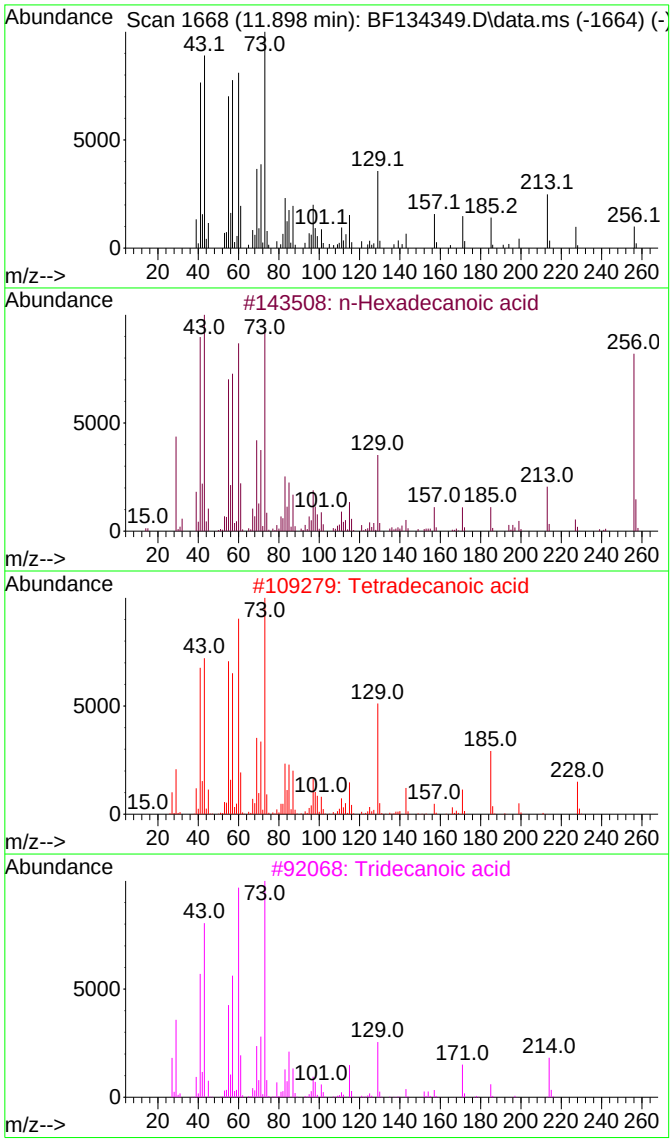
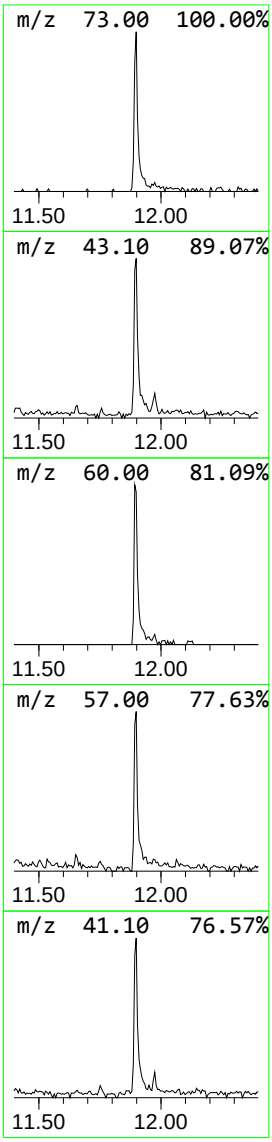
Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	5.52 ng	134482	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Data File : BF134349.D
Acq On : 18 Jul 2023 21:23
Operator : CG\JU
Sample : 03597-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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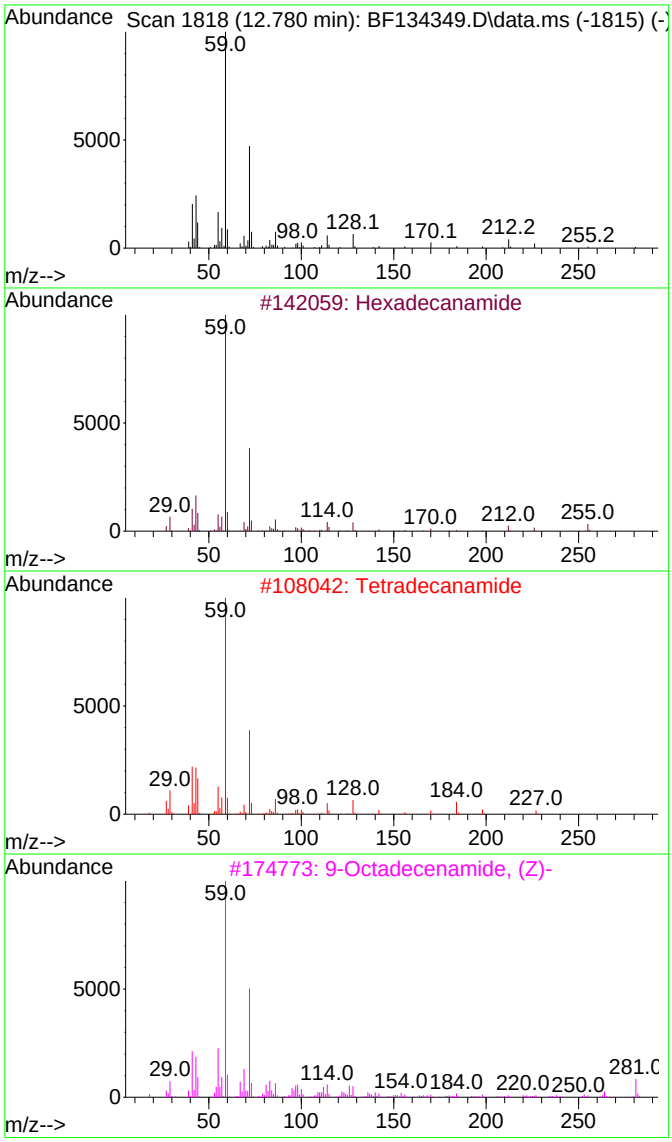
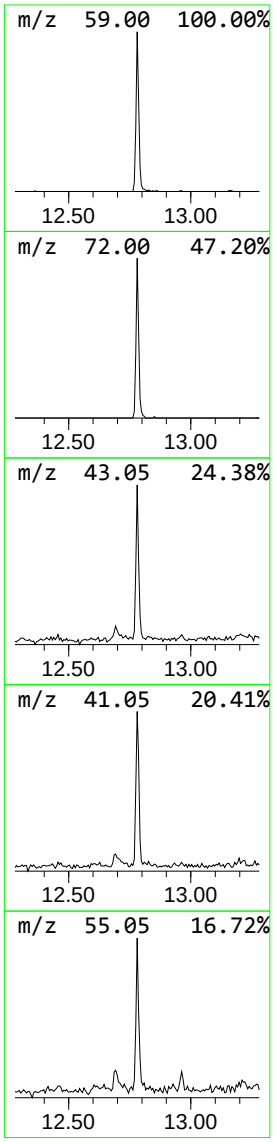
Peak Number 2 Hexadecanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.780	5.98 ng	115620	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
4	Octanamide	143	C8H17NO	000629-01-6	64
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64





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Acq On : 18 Jul 2023 21:23
Operator : CG\JU
Sample : 03597-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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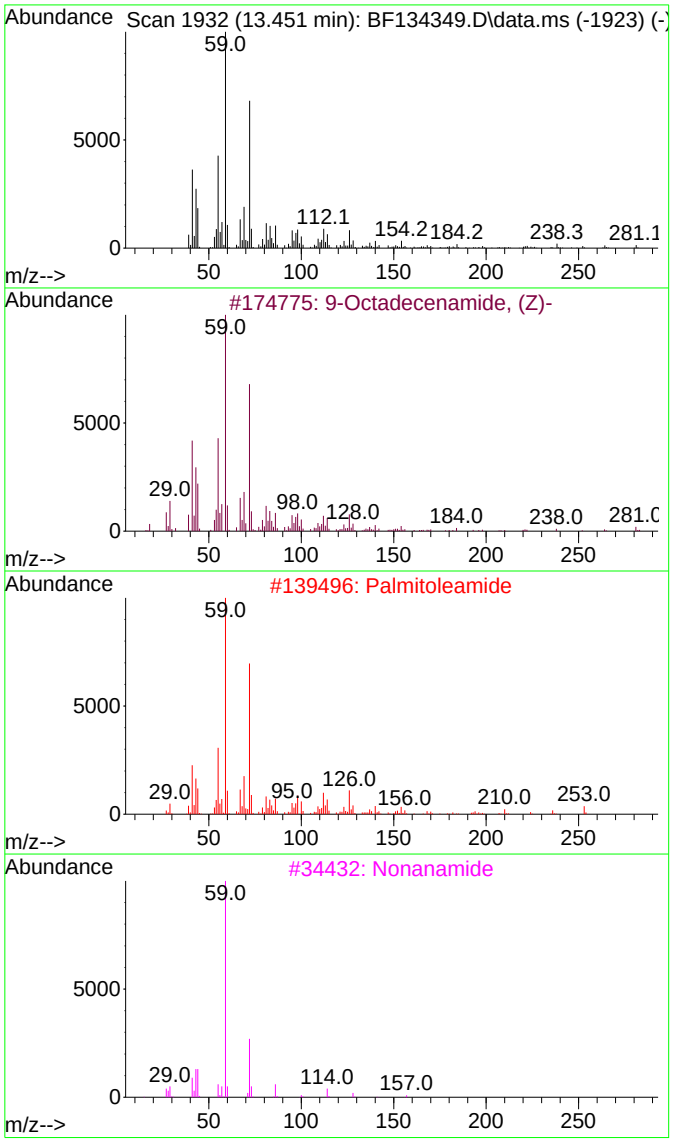
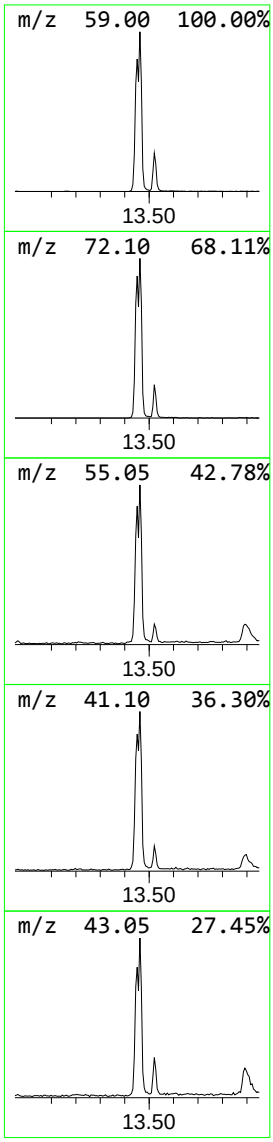
Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	33.31 ng	644215	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Palmitoleamide	253	C16H31NO	106010-22-4	83
3	Nonanamide	157	C9H19NO	001120-07-6	64
4	Octanamide	143	C8H17NO	000629-01-6	64
5	Silane, hexyl-	116	C6H16Si	001072-14-6	50





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Operator : CG\JU
Sample : 03597-16
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Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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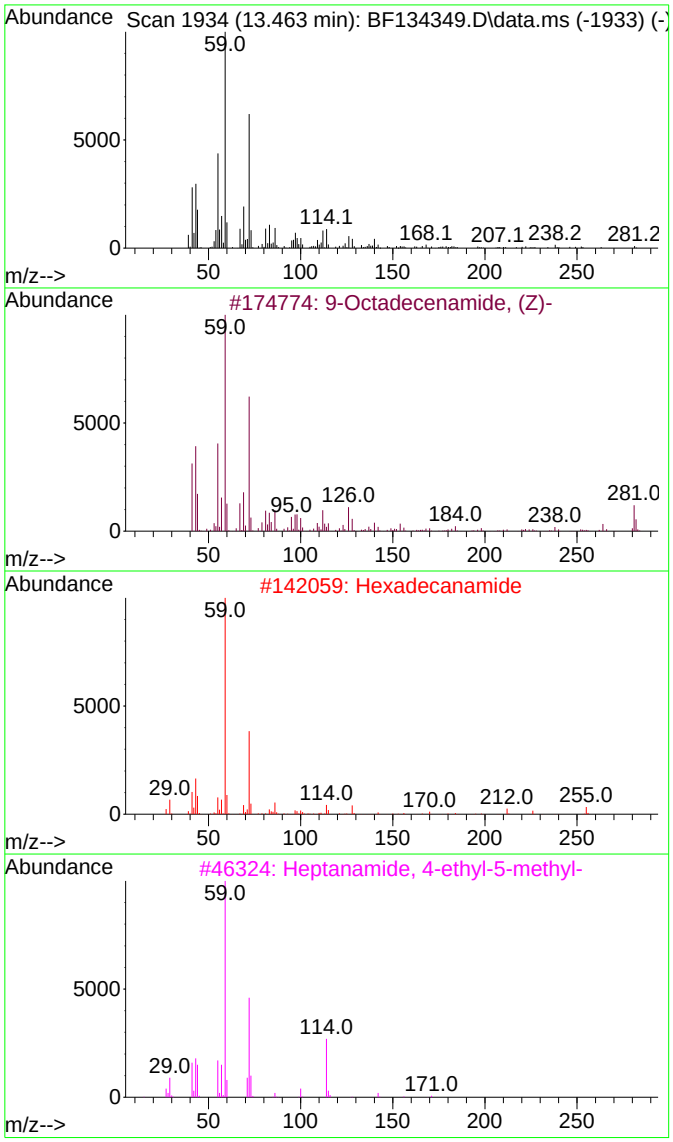
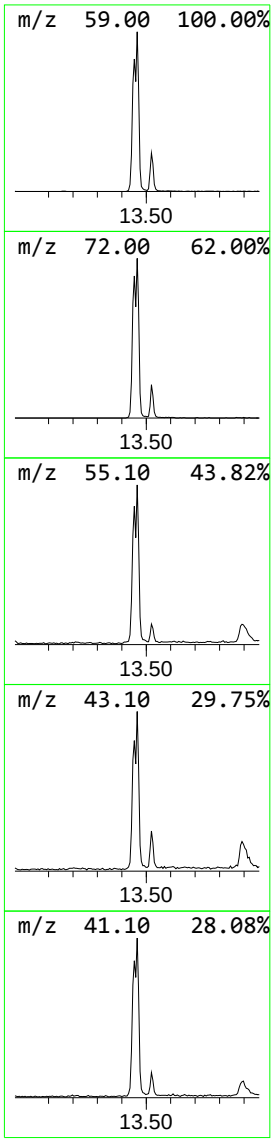
Peak Number 4 Heptanamide, 4-ethyl-5-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	25.56 ng	494299	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	78
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
4	7-Nonenamide	155	C9H17NO	090949-53-4	72
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134349.D
Acq On : 18 Jul 2023 21:23
Operator : CG\JU
Sample : 03597-16
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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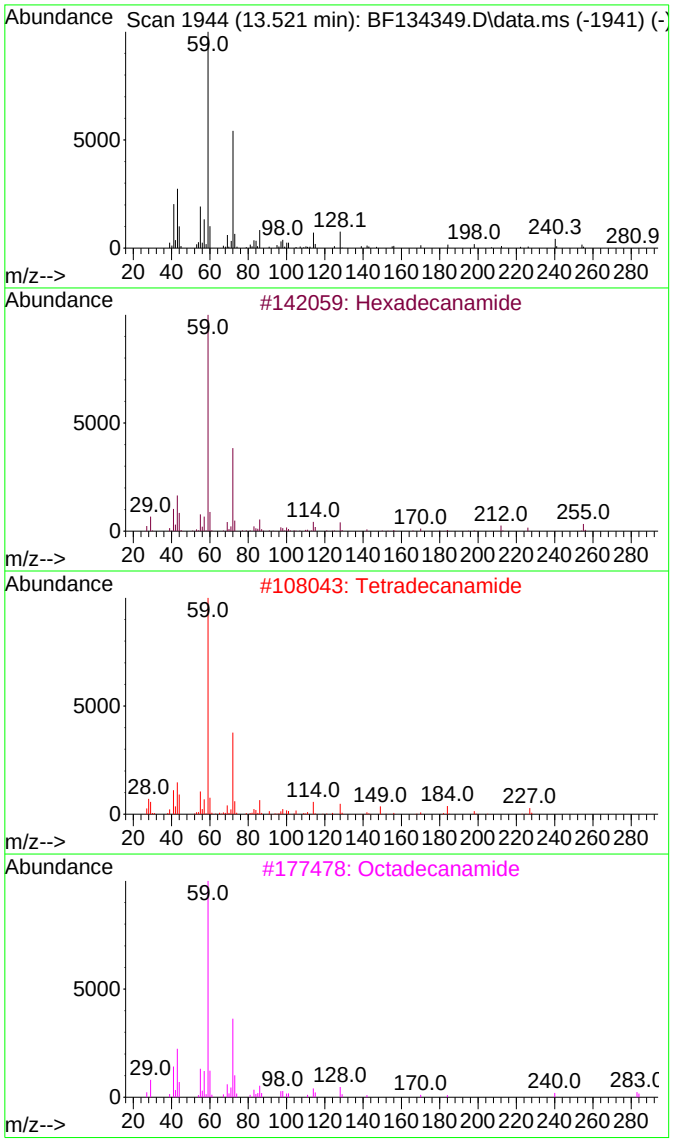
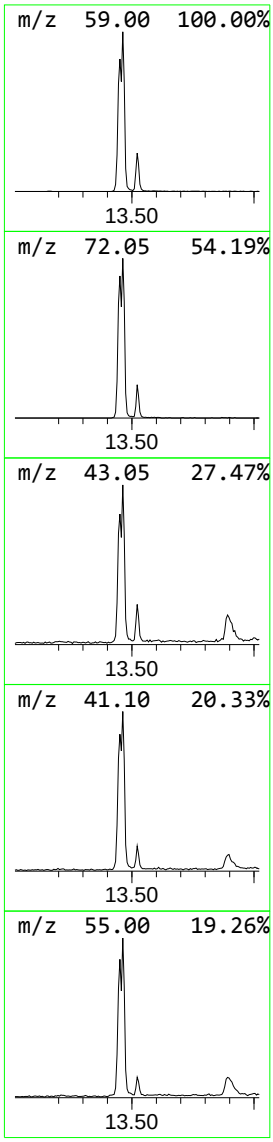
Peak Number 5 Tetradecanamide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.521	4.85 ng	93785	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	86
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	Octadecanamide	283	C18H37NO	000124-26-5	72
4	Nonadecanamide	297	C19H39NO	058185-32-3	64
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	64





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Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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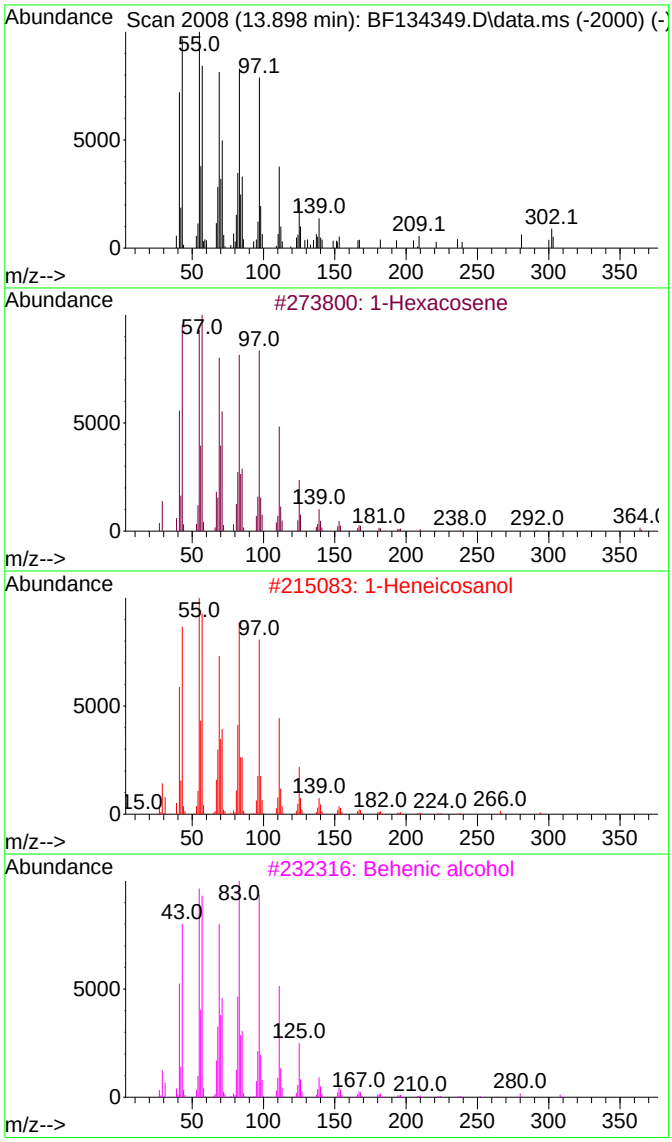
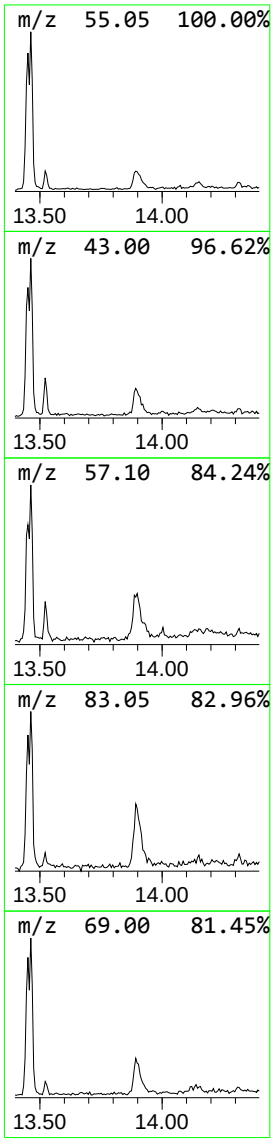
Peak Number 6 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	8.43 ng	163124	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





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Instrument :
BNA_F
ClientSampleId :
RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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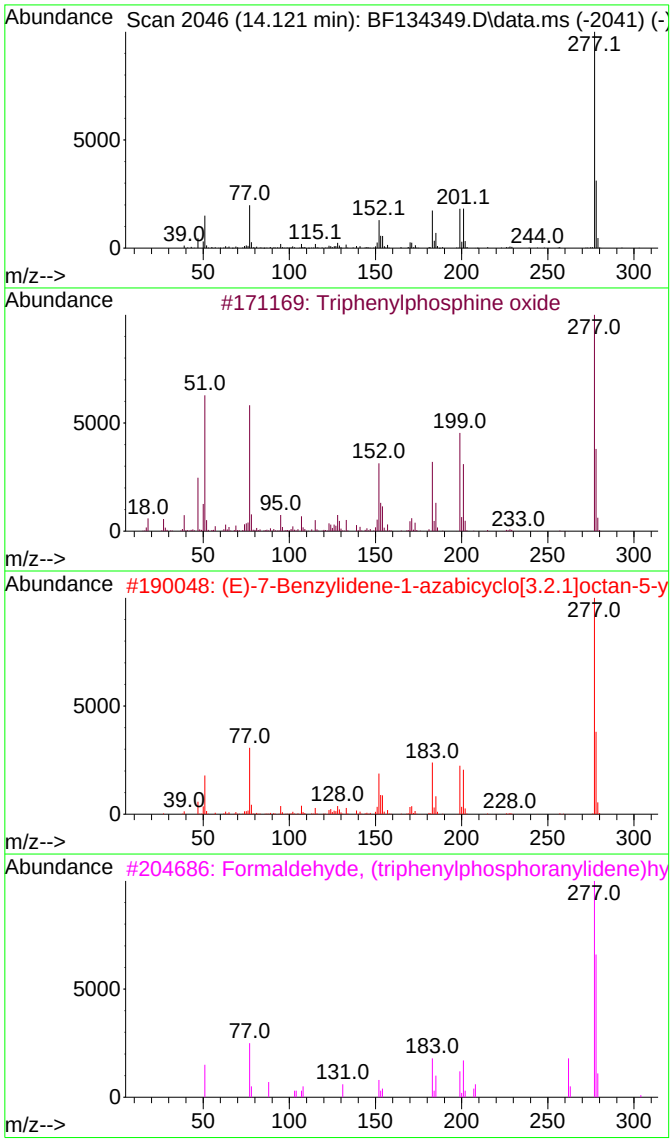
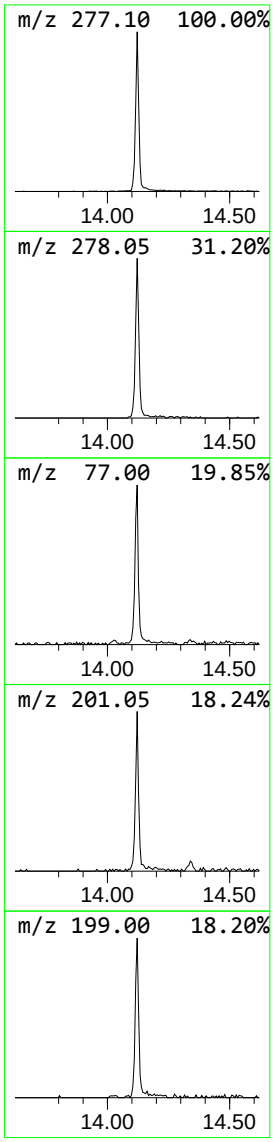
Peak Number 7 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	15.83 ng	306157	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	53
4	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	50
5	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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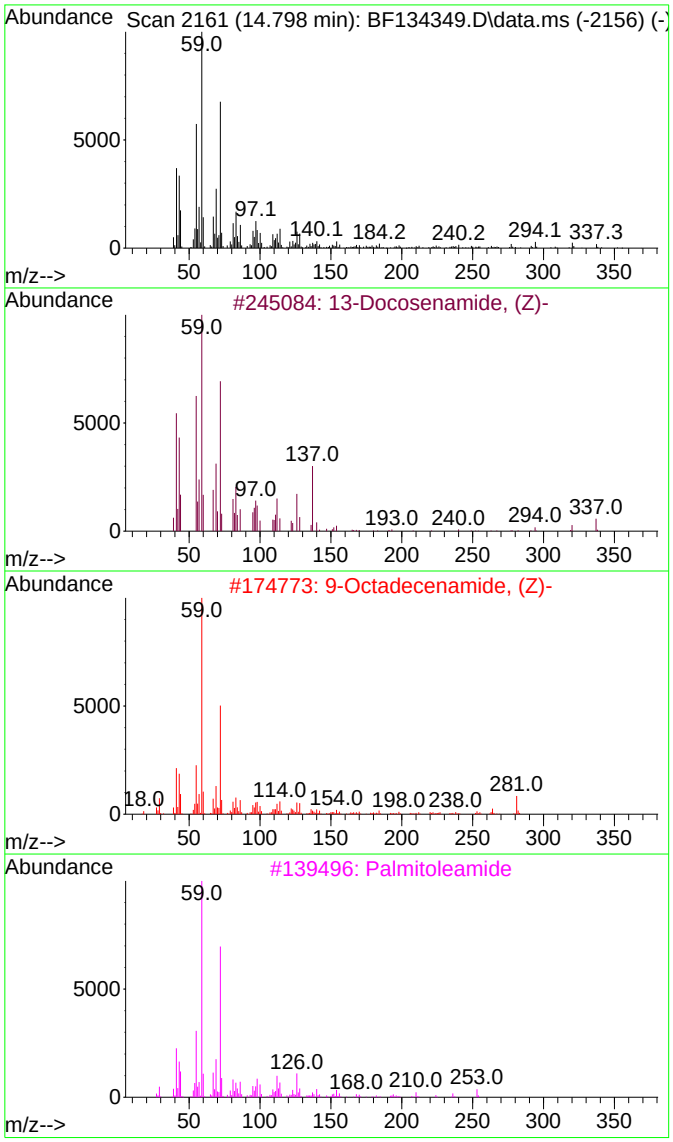
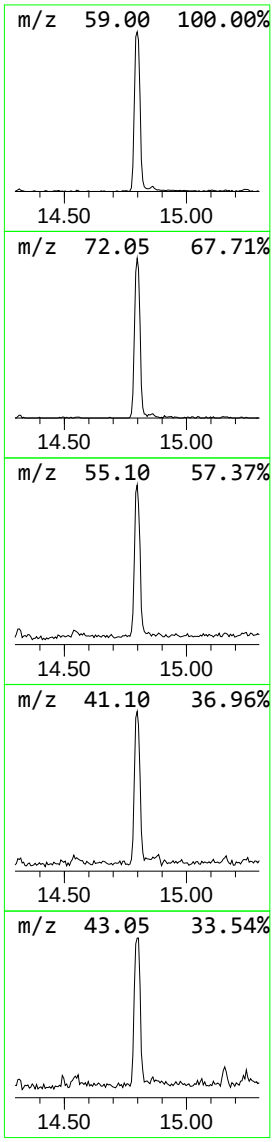
Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.798	28.25 ng	555869	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
3	Palmitoleamide	253	C16H31NO	106010-22-4	81
4	9-Octadecenamide	281	C18H35NO	003322-62-1	72
5	Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	43





Tentatively Identified Compound (LSC) summary

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Data File : BF134349.D
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RB-49-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	11.898	5.5	ng	134482	4	11.369	487465	20.0
Hexadecanamide	12.780	6.0	ng	115620	5	14.027	386813	20.0
9-Octadecenamid...	13.451	33.3	ng	644215	5	14.027	386813	20.0
Heptanamide, 4-...	13.463	25.6	ng	494299	5	14.027	386813	20.0
Tetradecanamide	13.521	4.8	ng	93785	5	14.027	386813	20.0
1-Hexacosene	13.898	8.4	ng	163124	5	14.027	386813	20.0
Triphenylphosph...	14.121	15.8	ng	306157	5	14.027	386813	20.0
13-Docosenamide...	14.798	28.3	ng	555869	6	15.533	393472	20.0