LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032725\
Data File : BF142123.D
Acq On : 27 Mar 2025 13:38
Operator : RC/JU
Sample : Q1644-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031925

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142123.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	571	576	593	rBV	825034	1218059	2.98%	1.216%
2	6.498	740	749	759	rBV	385827	727340	1.78%	0.726%
3	6.869	807	812	816	rBV	501679	631647	1.55%	0.631%
4	7.428	896	907	912	rBV	1336337	1870857	4.58%	1.868%
5	7.892	971	986	997	rBV	856475	2464736	6.03%	2.462%
6	7.986	997	1002	1007	rVV	346178	455562	1.11%	0.455%
7	8.151	1025	1030	1035	rBV	647824	831984	2.04%	0.831%
8	8.475	1079	1085	1099	rVB	4658547	7904366	19.35%	7.894%
9	9.228	1207	1213	1218	rBV	2910526	3607307	8.83%	3.603%
10	9.551	1258	1268	1277	rBV	14214301	40858903	100.00%	40.806%
11	9.628	1277	1281	1285	rVB	1642138	2326074	5.69%	2.323%
12	9.910	1325	1329	1336	rVB	786815	984573	2.41%	0.983%
13	10.616	1445	1449	1456	rVV2	420824	576032	1.41%	0.575%
14	10.704	1459	1464	1471	rVB	2057877	2656189	6.50%	2.653%
15	11.392	1577	1581	1589	rBV	748515	962880	2.36%	0.962%
16	11.951	1666	1676	1692	rVB	4366342	9701334	23.74%	9.689%
17	12.633	1785	1792	1797	rBV2	531299	1415025	3.46%	1.413%
18	12.739	1800	1810	1830	rVB	6794738	15433645	37.77%	15.414%
19	12.980	1846	1851	1862	rVB	2995685	3939287	9.64%	3.934%
20	14.033	2026	2030	2036	rVB	572437	726819	1.78%	0.726%
21	15.510	2275	2281	2292	rVB	520932	836169	2.05%	0.835%

Sum of corrected areas: 100128788

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032725\
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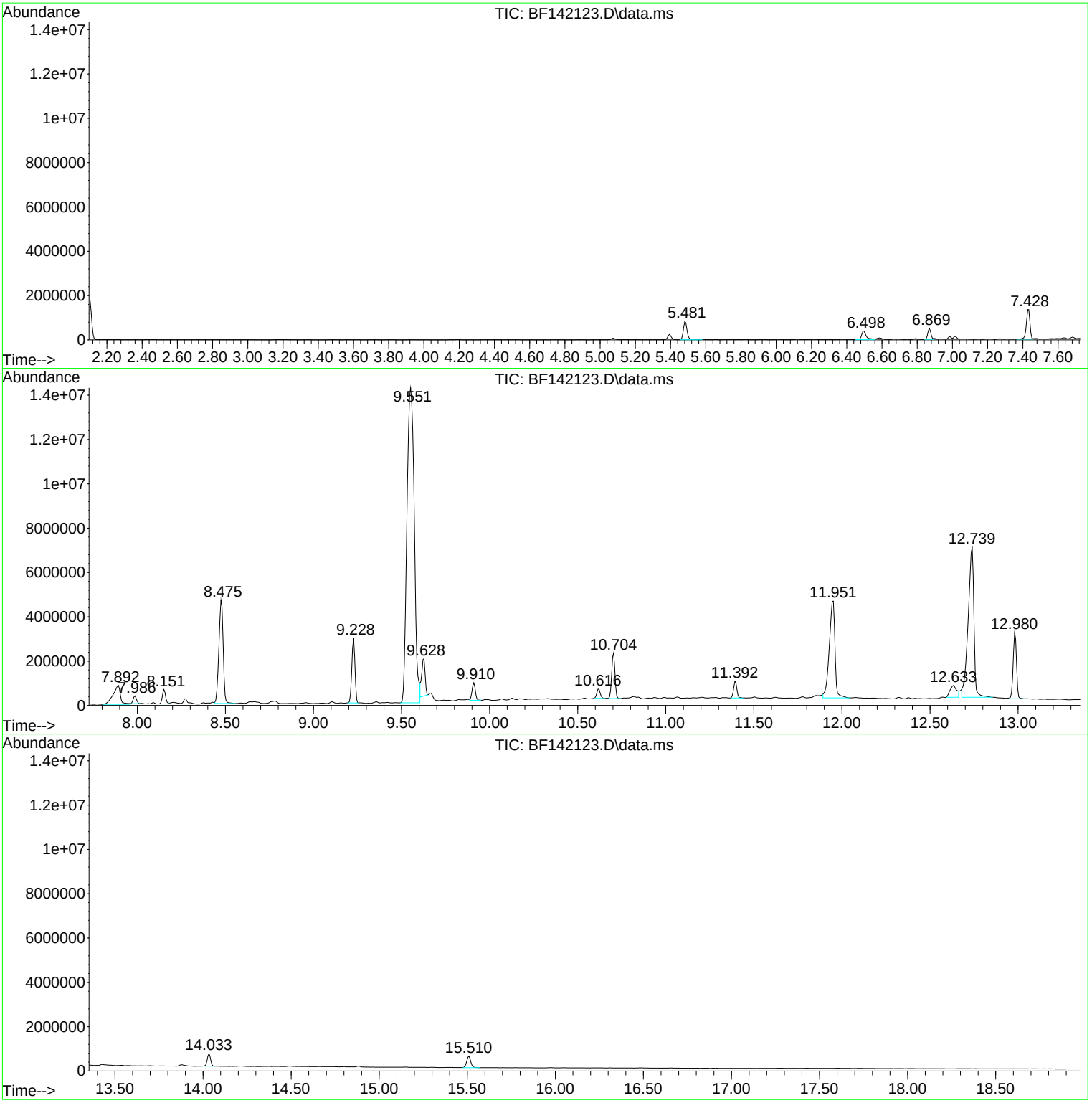
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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\BF032725\
Data File : BF142123.D
Acq On : 27 Mar 2025 13:38
Operator : RC/JU
Sample : Q1644-03
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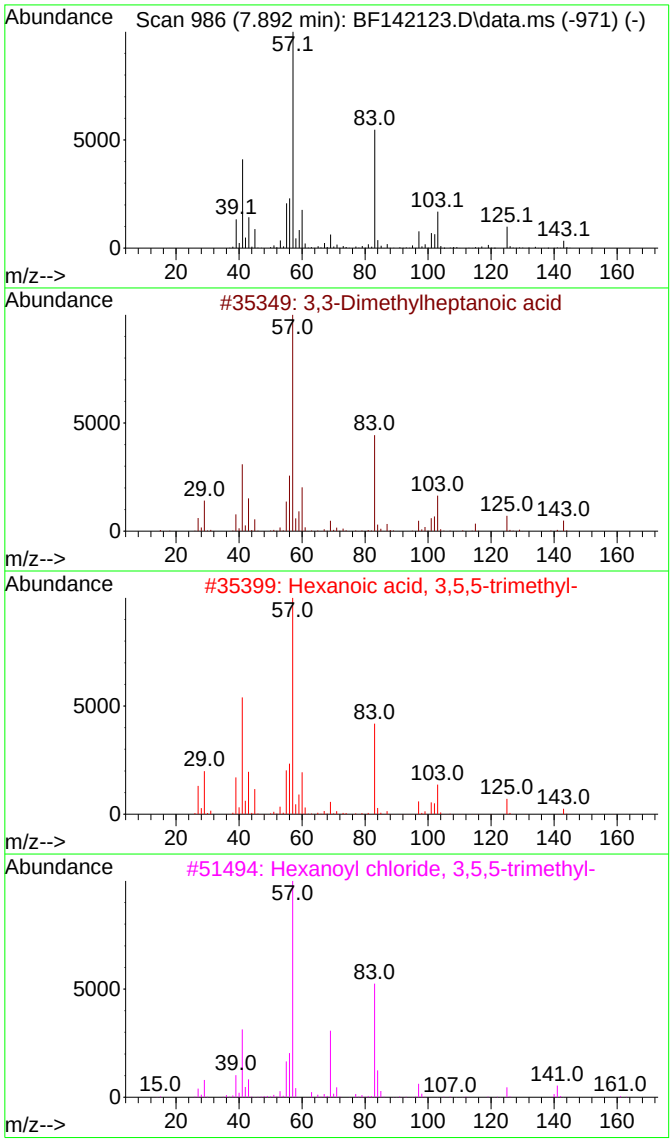
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

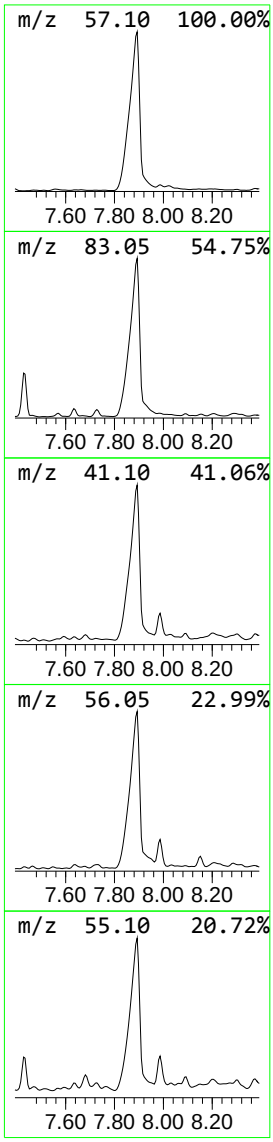
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3,3-Dimethylheptanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.892	59.25 ng	2464740	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	90
2	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
3	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	53
4	CH3C(O)OCH(CH3)CH2C(CH3)3	158	C9H18O2	060388-83-2	38
5	Propanoic acid, 2,2-dimethyl-, c...	184	C11H20O2	029878-49-7	32





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Data File : BF142123.D
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Operator : RC/JU
Sample : Q1644-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

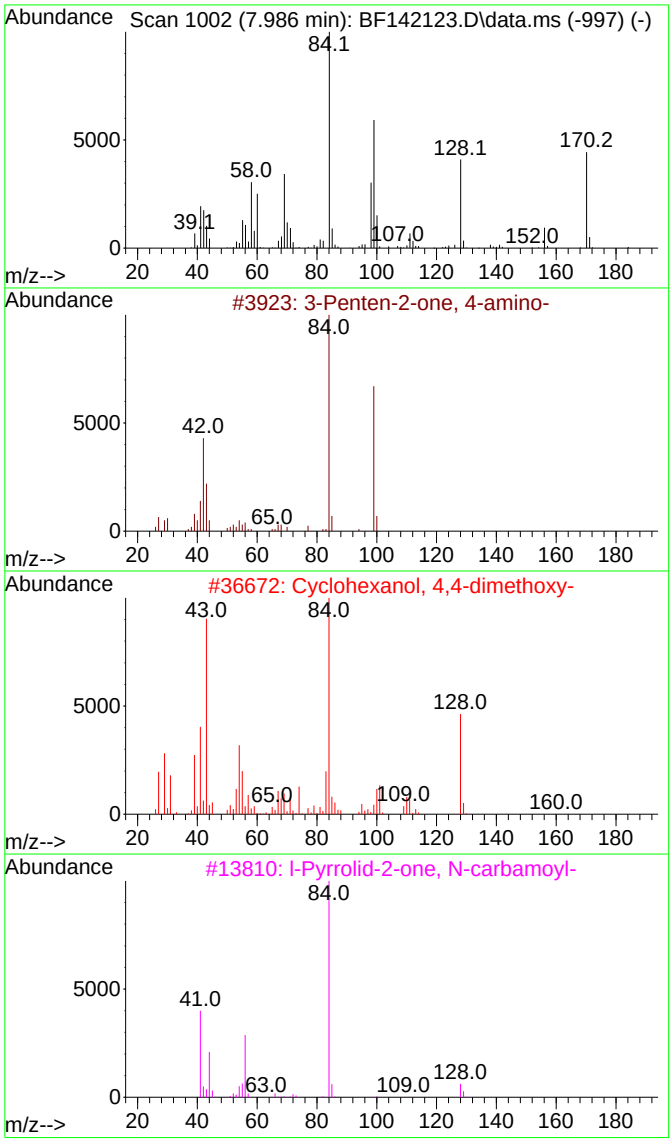
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

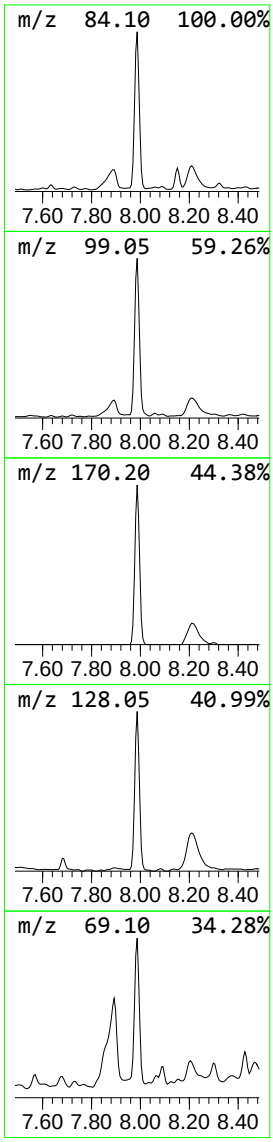
****

Peak Number 2 unknown7.986 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.986	10.95 ng	455562	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-amino-	99	C5H9NO	001118-66-7	35
2	Cyclohexanol, 4,4-dimethoxy-	160	C8H16O3	112906-44-2	32
3	l-Pyrrolid-2-one, N-carbamoyl-	128	C5H8N2O2	040451-67-0	25
4	[1-Cyclopropyl-2-(3-fluorophenox...	209	C12H16FNO	1000487-14-0	22
5	5-Methoxypyrrolidin-2-one	115	C5H9NO2	063853-74-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032725\
Data File : BF142123.D
Acq On : 27 Mar 2025 13:38
Operator : RC/JU
Sample : Q1644-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

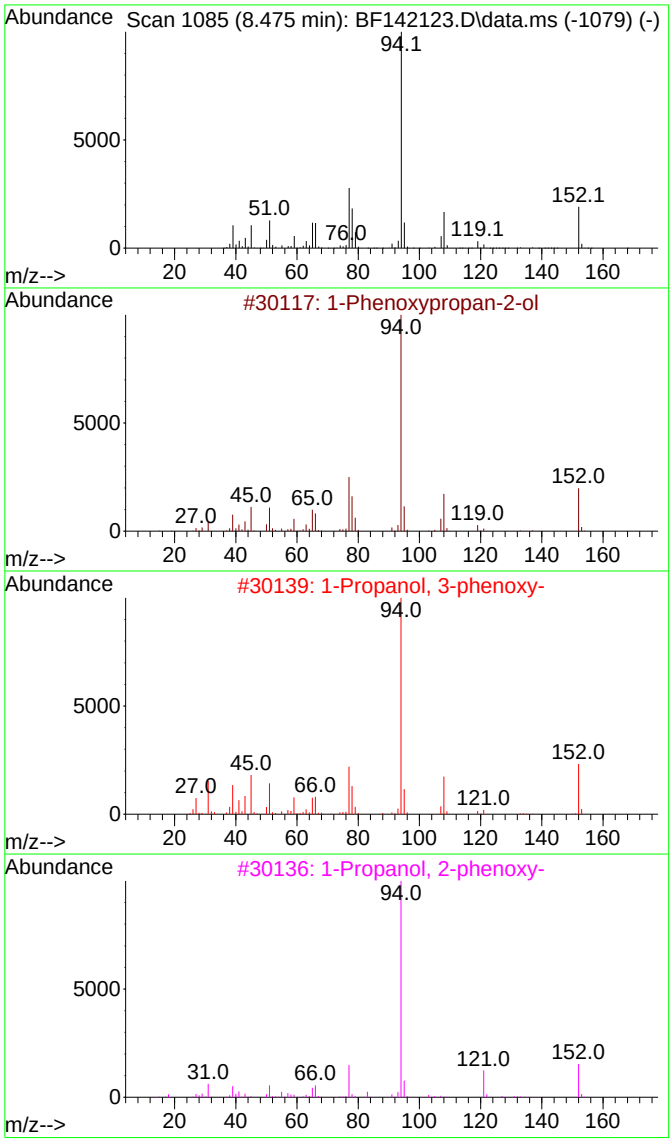
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

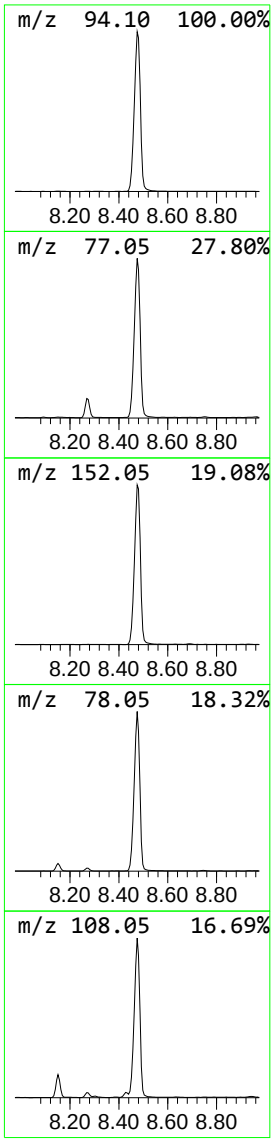
****

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	190.01 ng	7904370	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
5	DL-Gabaculine	139	C7H9NO2	059556-18-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032725\
Data File : BF142123.D
Acq On : 27 Mar 2025 13:38
Operator : RC/JU
Sample : Q1644-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031925

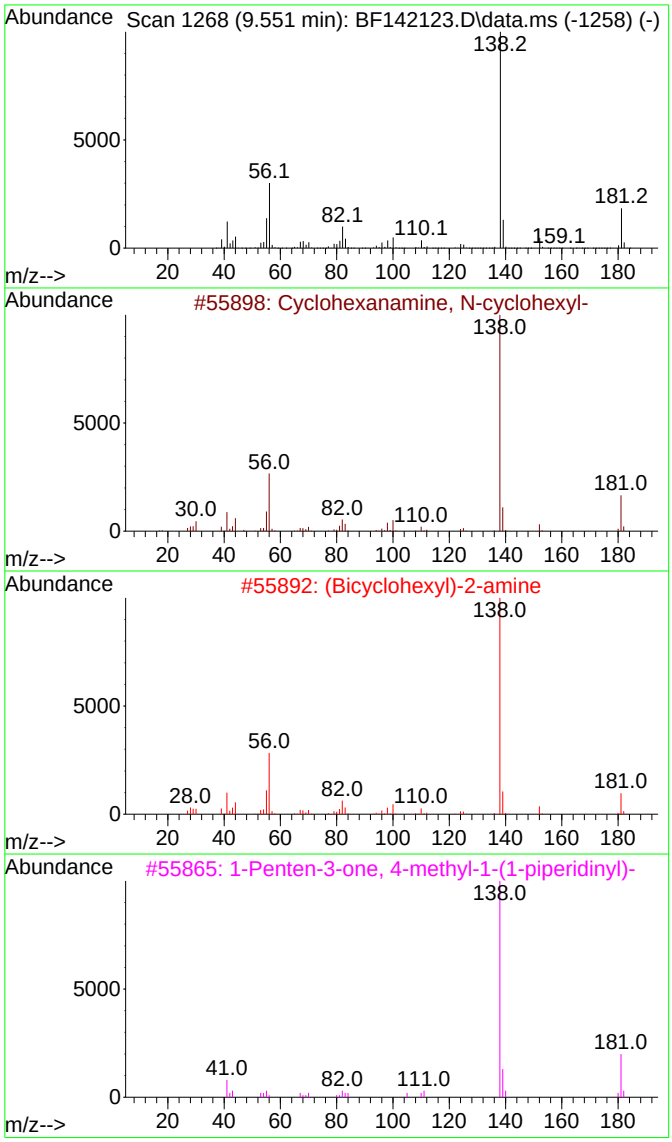
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

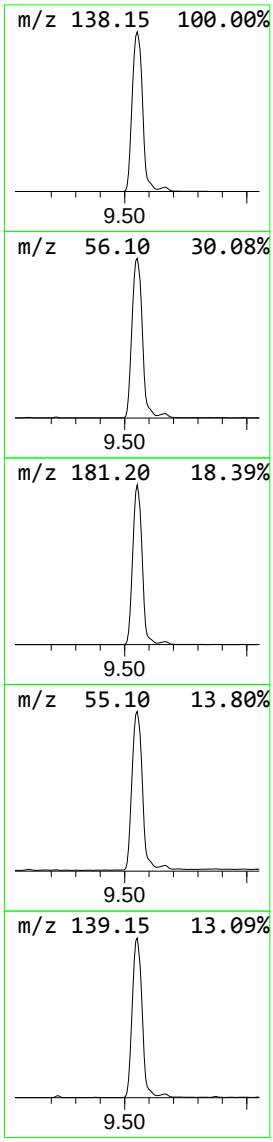
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexanamine, N-cyclohexyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.551	829.98 ng	40858900	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	95
2	(Bicyclohexyl)-2-amine	181	C12H23N	006283-14-3	91
3	1-Penten-3-one, 4-methyl-1-(1-pi...	181	C11H19NO	013606-83-2	58
4	4,6-Dimethyl-2-pyrimidinylhydrazine	138	C6H10N4	023906-13-0	50
5	Gephyrotoxin 181b	181	C12H23N	120030-08-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032725\
Data File : BF142123.D
Acq On : 27 Mar 2025 13:38
Operator : RC/JU
Sample : Q1644-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
031925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

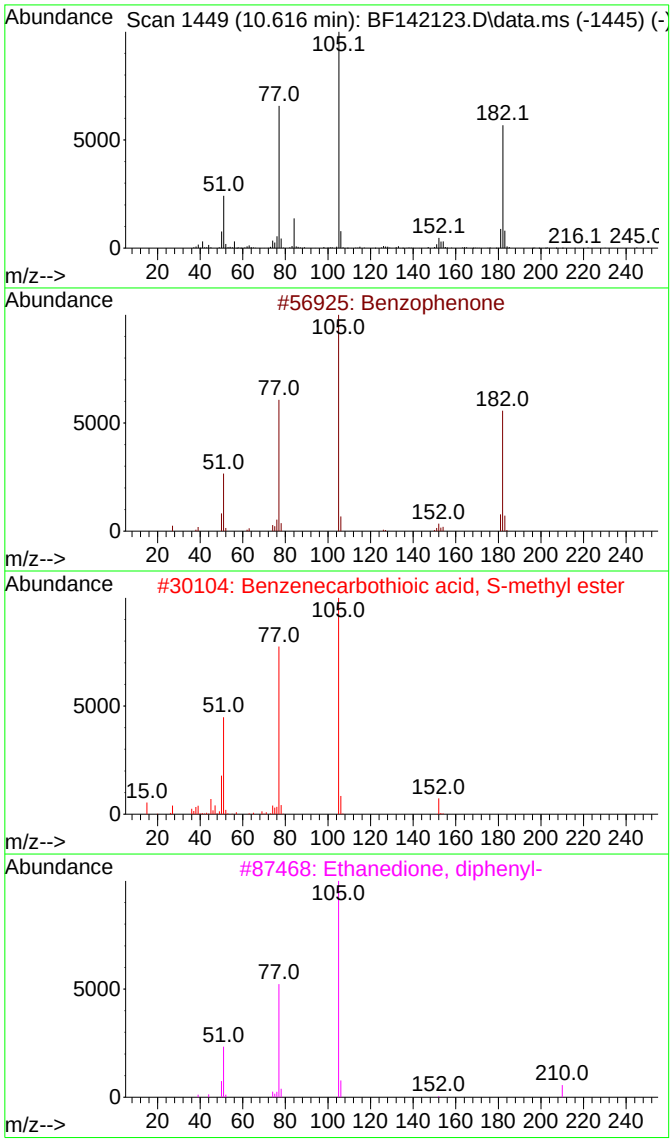
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

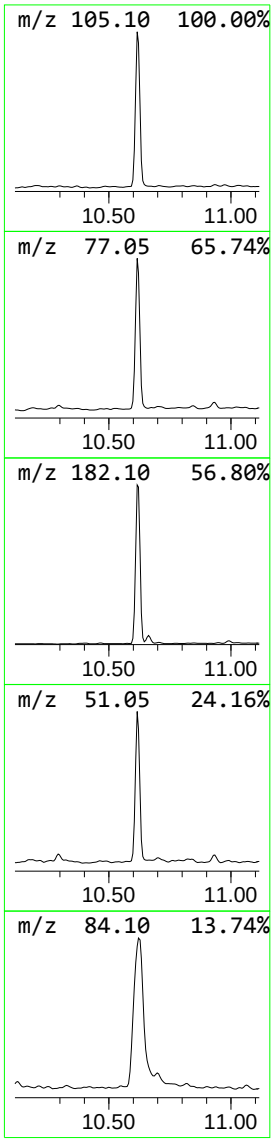
****

Peak Number 5 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	11.70 ng	576032	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	43
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43
5	Butanenitrile, 2,3-bis(benzoylox...	335	C18H13N3O4	1000269-66-6	43





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Instrument :
BNA_F
ClientSampleId :
031925

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

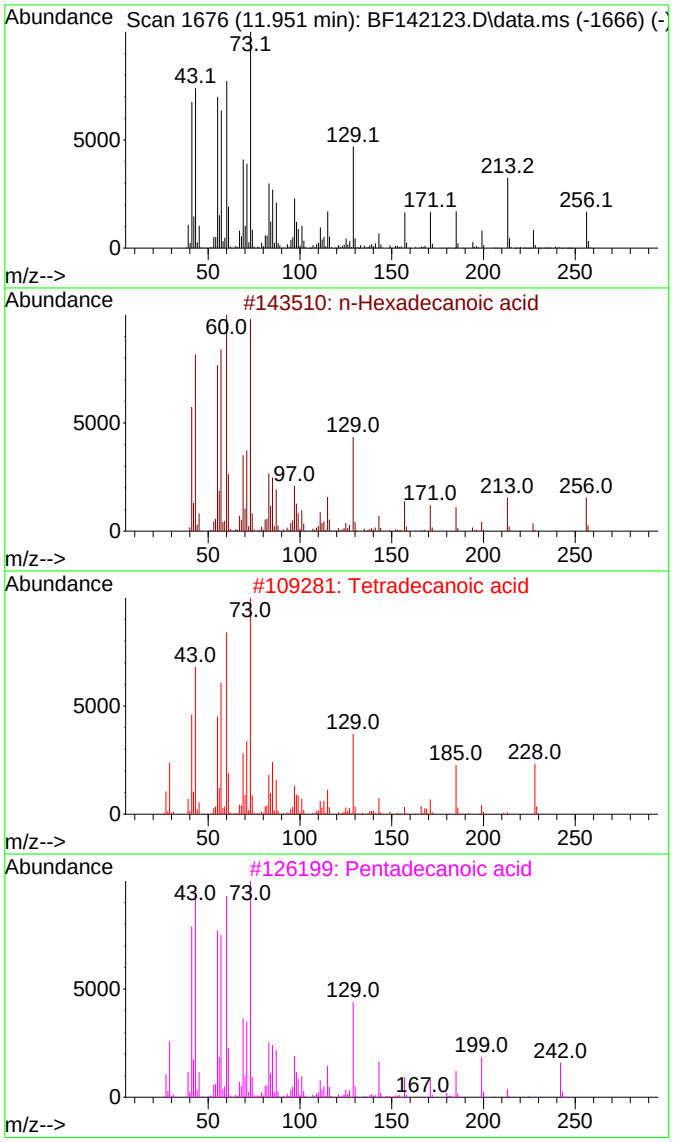
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

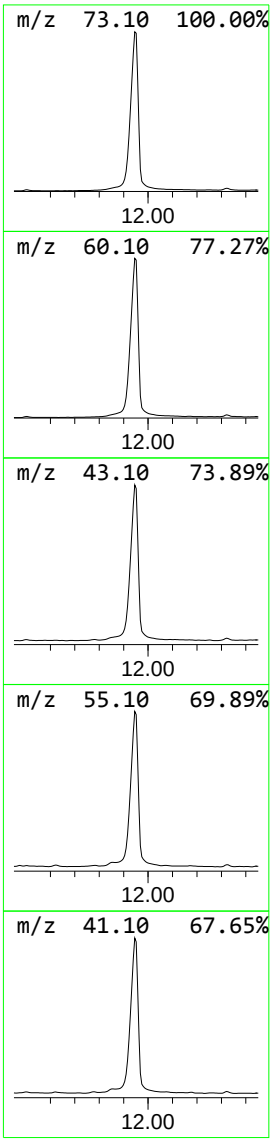
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	201.51 ng	9701330	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





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Sample : Q1644-03
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

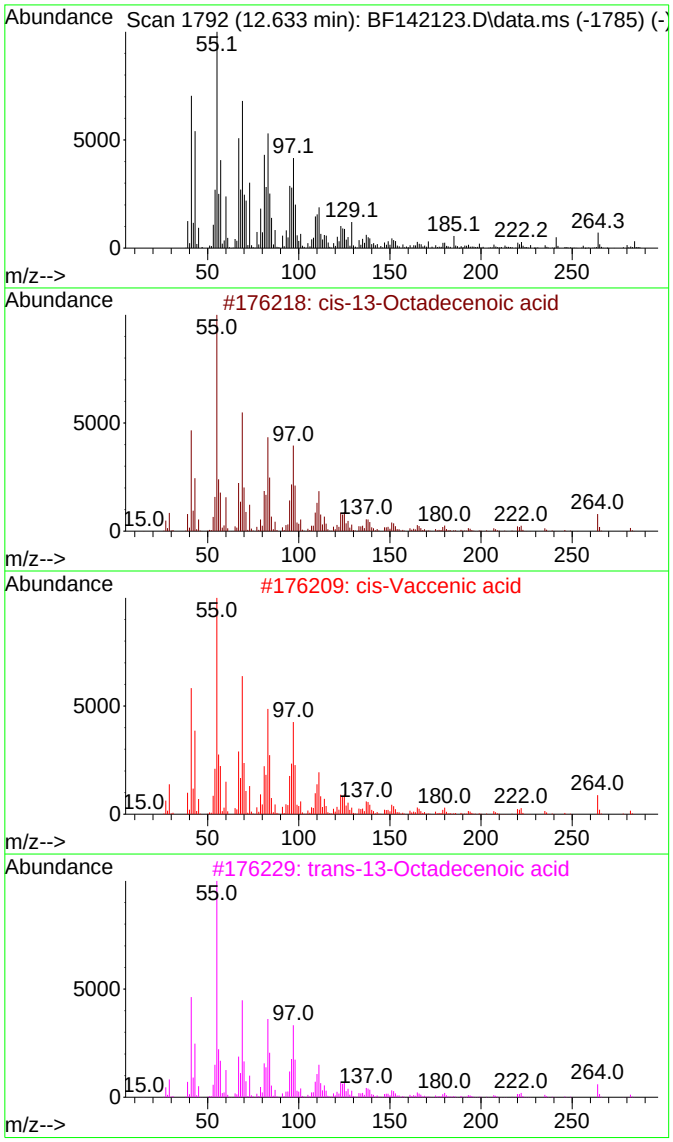
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

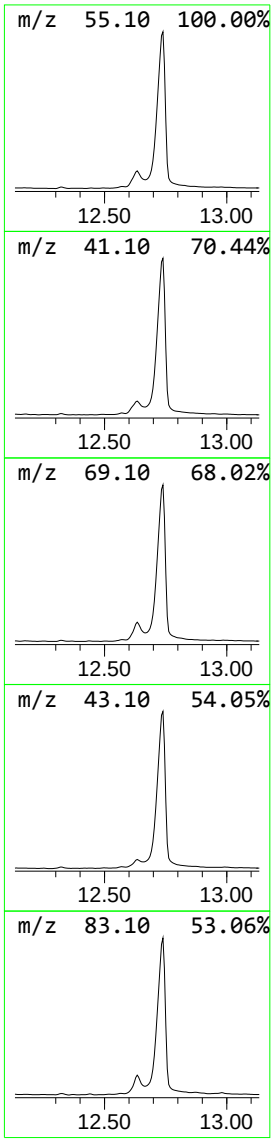
****

Peak Number 7 cis-13-Octadecenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	29.39 ng	1415030	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	97
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	96
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
4	Oxacyclopentadecan-2-one	226	C14H26O2	003537-83-5	83
5	cis-10-Nonadecenoic acid	296	C19H36O2	073033-09-7	76





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TIC Library : C:\Database\NIST20.L
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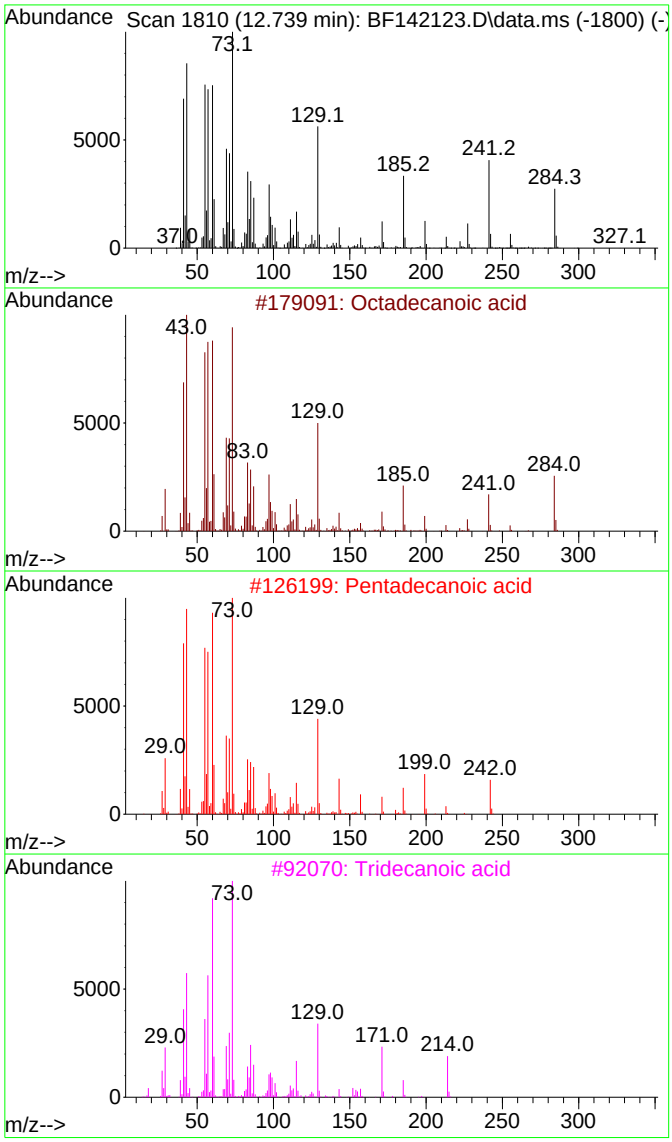
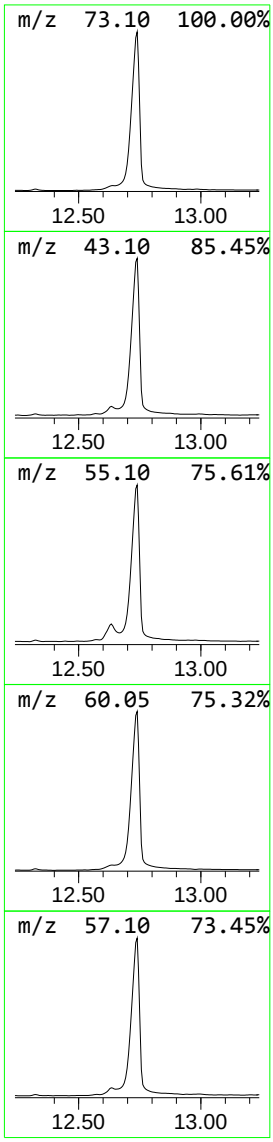
****

Peak Number 8 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	424.69 ng	15433600	Chrysene-d12	14.033

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	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Tentatively Identified Compound (LSC) summary

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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
3,3-Dimethylhep...	7.892	59.3	ng	2464740	2	8.151	831984	20.0
unknown7.986	7.986	10.9	ng	455562	2	8.151	831984	20.0
1-Phenoxypropan...	8.475	190.0	ng	7904370	2	8.151	831984	20.0
Cyclohexanamine...	9.551	830.0	ng	40858900	3	9.910	984573	20.0
Benzophenone	10.616	11.7	ng	576032	3	9.910	984573	20.0
n-Hexadecanoic ...	11.951	201.5	ng	9701330	4	11.392	962880	20.0
cis-13-Octadece...	12.633	29.4	ng	1415030	4	11.392	962880	20.0
Octadecanoic acid	12.739	424.7	ng	15433600	5	14.033	726819	20.0