LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139188.D
Acq On : 27 Aug 2024 15:48
Operator : RC/JU
Sample : P3732-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-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-BF082724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139188.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	8	16	23	rVB	1361923	2165552	94.89%	12.083%
2	3.387	214	220	232	rBV	46158	104254	4.57%	0.582%
3	5.110	503	513	526	rVB	107156	165847	7.27%	0.925%
4	5.510	574	581	586	rBV	1553969	2152112	94.30%	12.008%
5	6.516	745	752	757	rBV	1529057	2197954	96.31%	12.264%
6	6.710	780	785	798	rBV	56278	73741	3.23%	0.411%
7	6.893	811	816	821	rBV	403553	494391	21.66%	2.759%
8	7.451	905	911	916	rBV	1055482	1347490	59.05%	7.519%
9	7.704	950	954	959	rVB	29677	33985	1.49%	0.190%
10	8.169	1028	1033	1038	rBV	481465	610245	26.74%	3.405%
11	8.481	1081	1086	1097	rBV	106813	135565	5.94%	0.756%
12	9.245	1210	1216	1221	rBV	1864106	2282079	100.00%	12.734%
13	9.922	1326	1331	1336	rVB	550523	672474	29.47%	3.752%
14	10.022	1342	1348	1356	rBV	327428	496435	21.75%	2.770%
15	10.710	1460	1465	1478	rBV	1122383	1393203	61.05%	7.774%
16	11.410	1579	1584	1590	rBV	497531	609700	26.72%	3.402%
17	11.933	1668	1673	1683	rBV2	55044	82185	3.60%	0.459%
18	12.992	1848	1853	1858	rBV	1474450	1875534	82.19%	10.465%
19	13.898	2001	2007	2022	rBV	63219	125096	5.48%	0.698%
20	14.045	2027	2032	2045	rVB	390813	495594	21.72%	2.765%
21	15.516	2276	2282	2288	rBV	272511	408348	17.89%	2.279%

Sum of corrected areas: 17921784

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
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Operator : RC/JU
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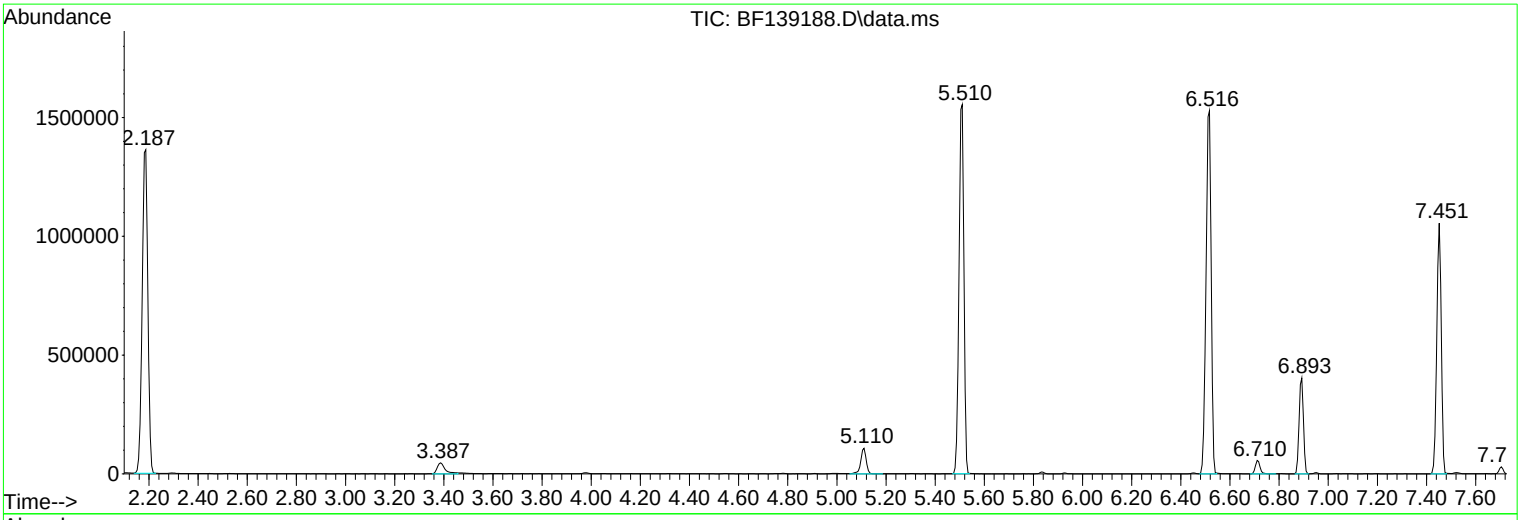
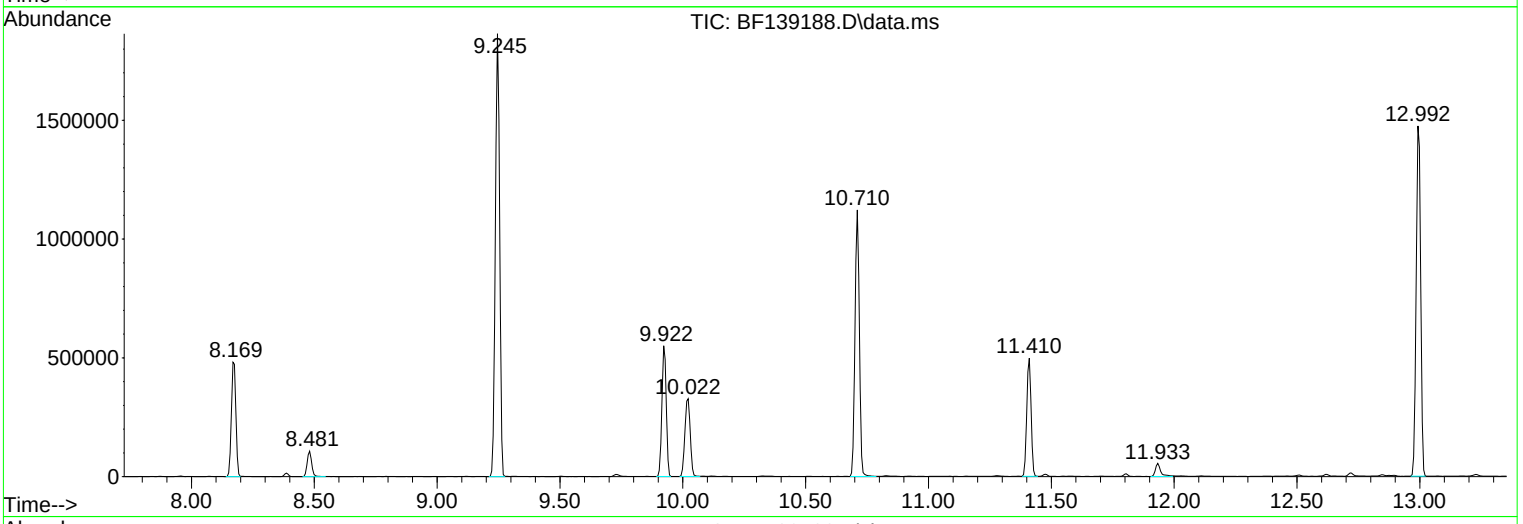
Misc :
ALS Vial : 15 Sample Multiplier: 1

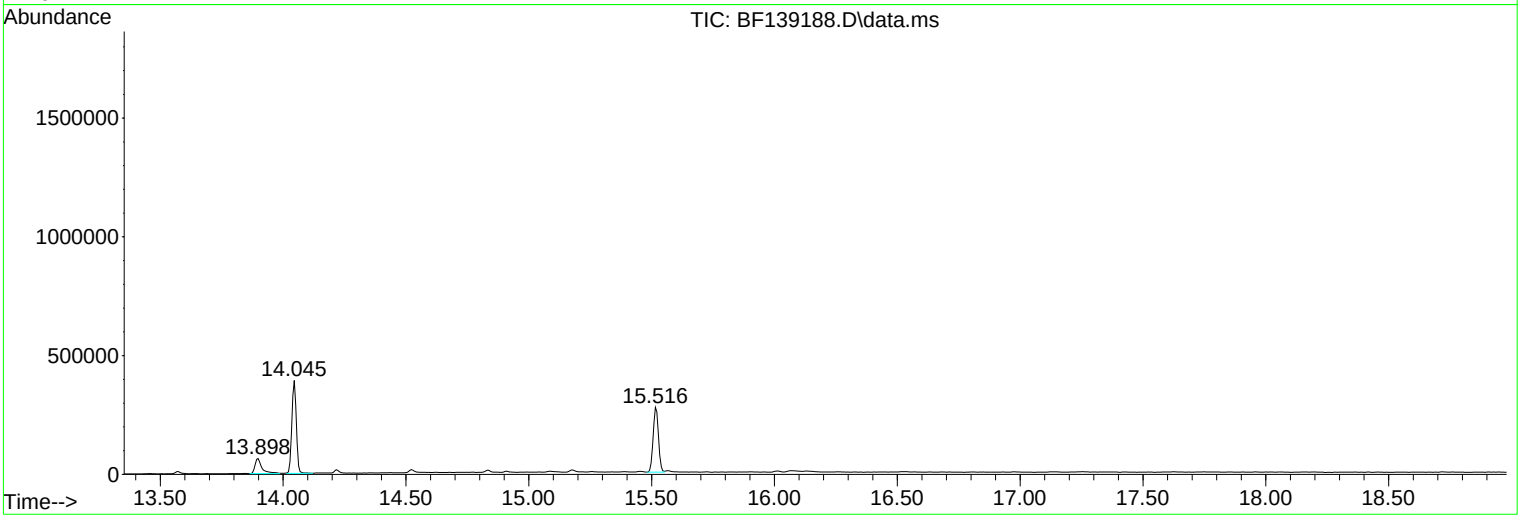
Instrument :
BNA_F
ClientSampleId :
UI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.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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Operator : RC/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

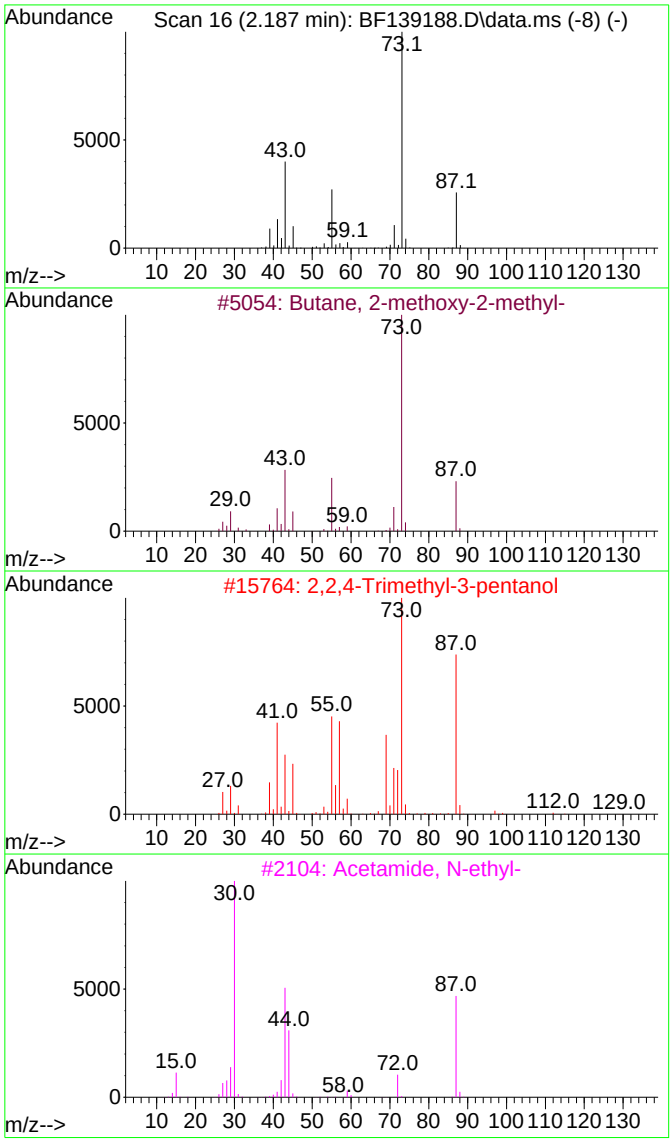
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

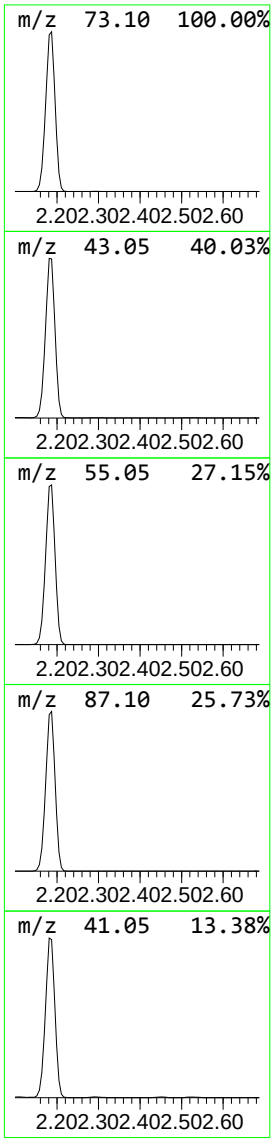
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	87.60 ng	2165550	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : RC/JU
Sample : P3732-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

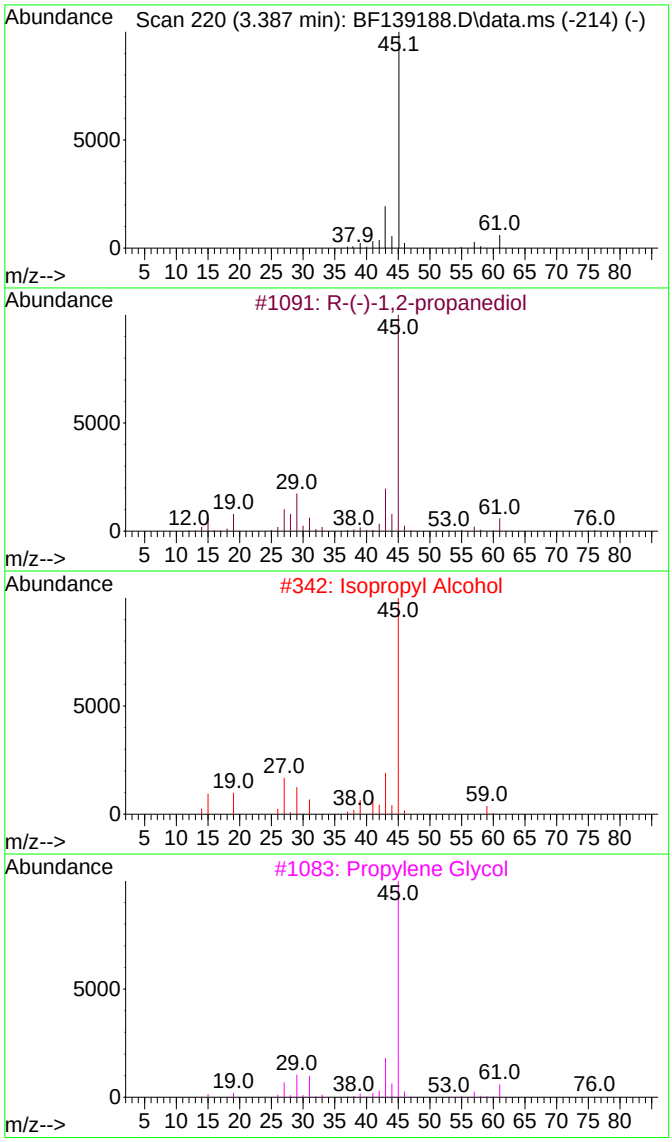
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

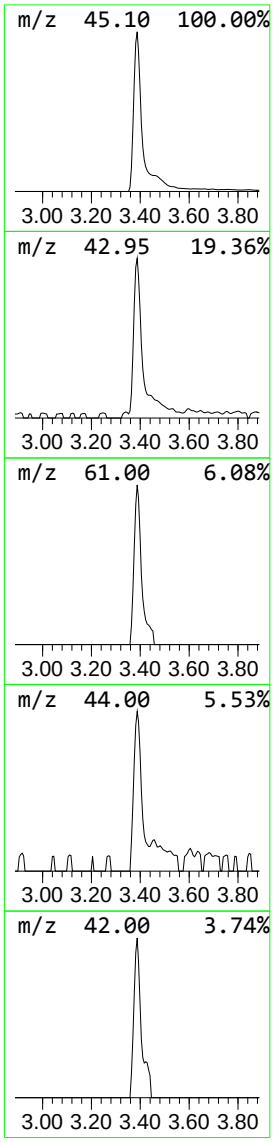
****

Peak Number 2 unknown3.387 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	4.22 ng	104254	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Formamide	45	CH3NO	000075-12-7	5
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	4





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Data File : BF139188.D
Acq On : 27 Aug 2024 15:48
Operator : RC/JU
Sample : P3732-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-5

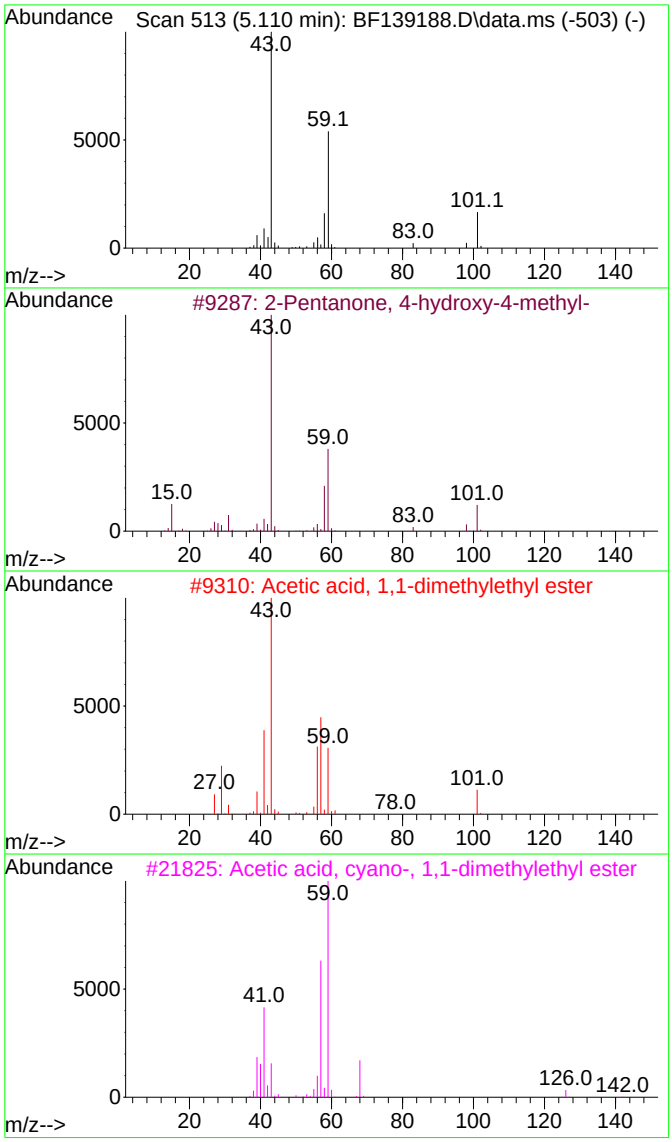
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

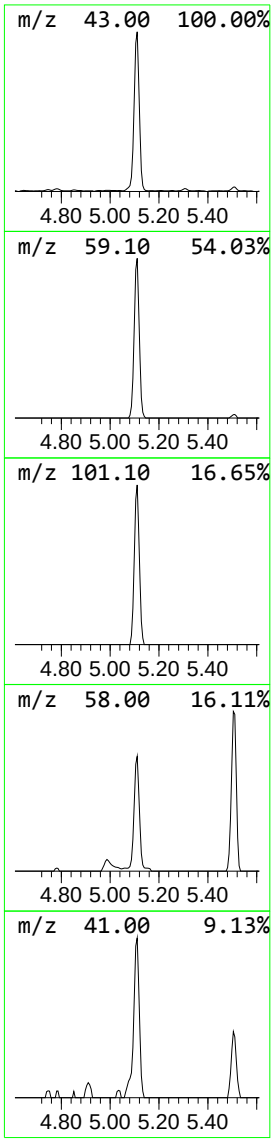
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	6.71 ng	165847	1,4-Dichlorobenzene-d4	6.893

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	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Acetone	58	C3H6O	000067-64-1	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
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Acq On : 27 Aug 2024 15:48
Operator : RC/JU
Sample : P3732-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

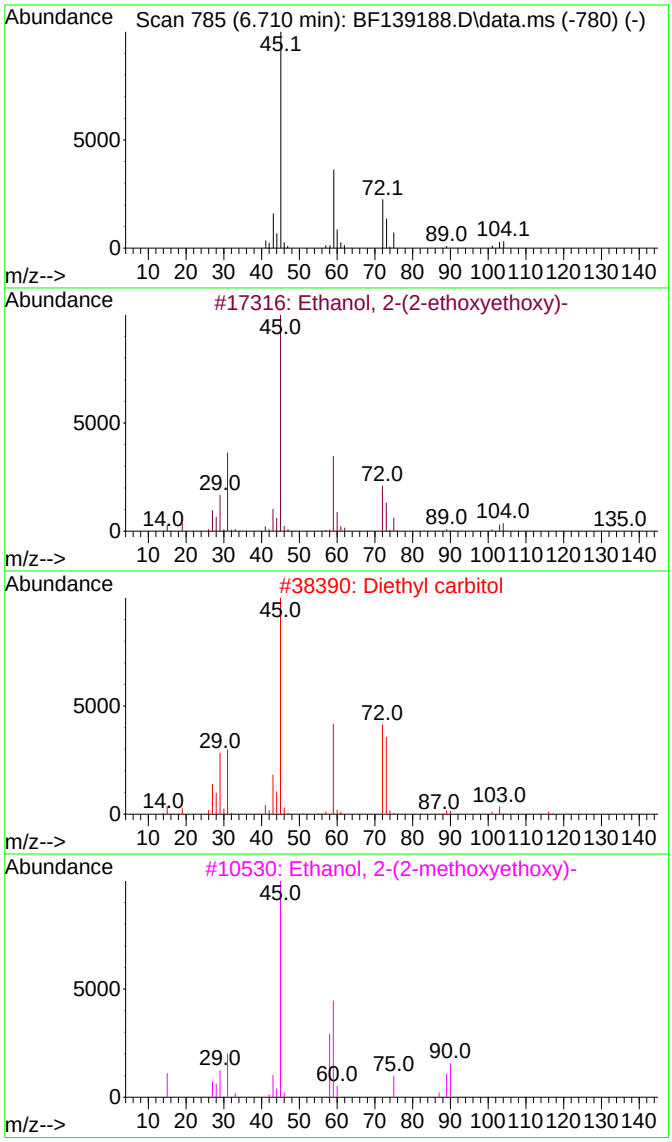
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

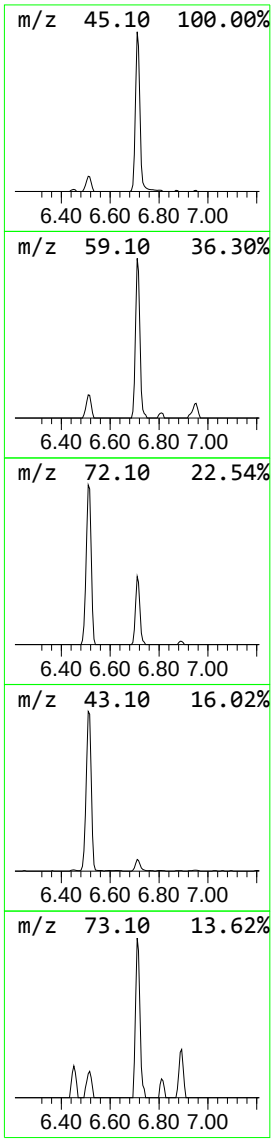
****

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.710	2.98 ng	73741	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	78
3	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	40
5	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082724\
Data File : BF139188.D
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Operator : RC/JU
Sample : P3732-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

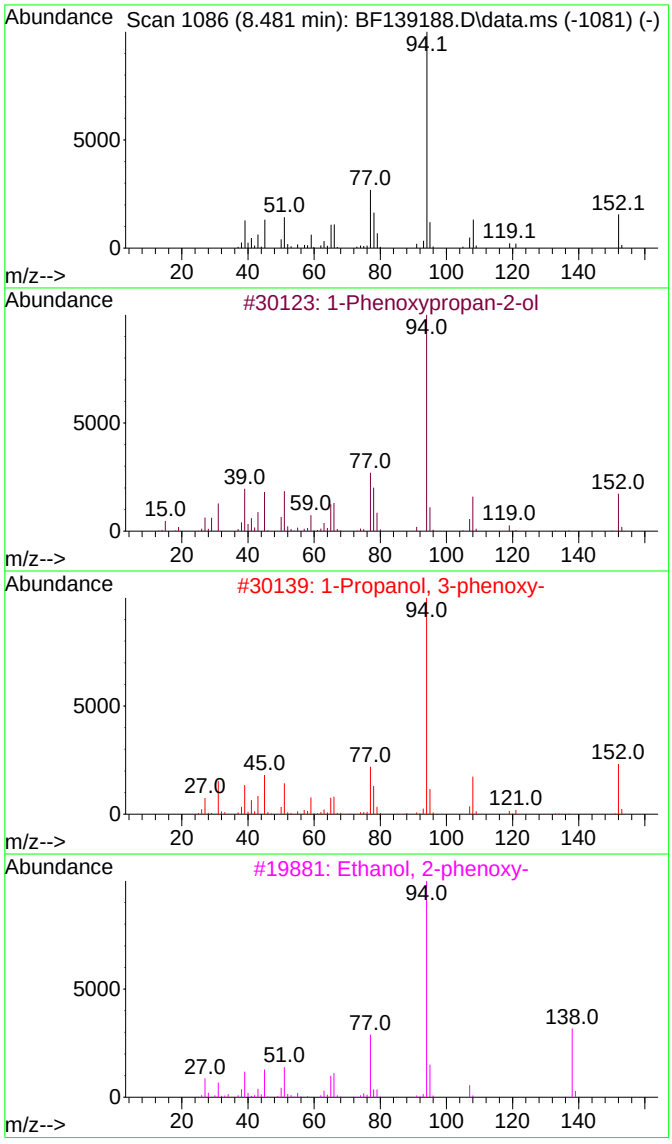
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

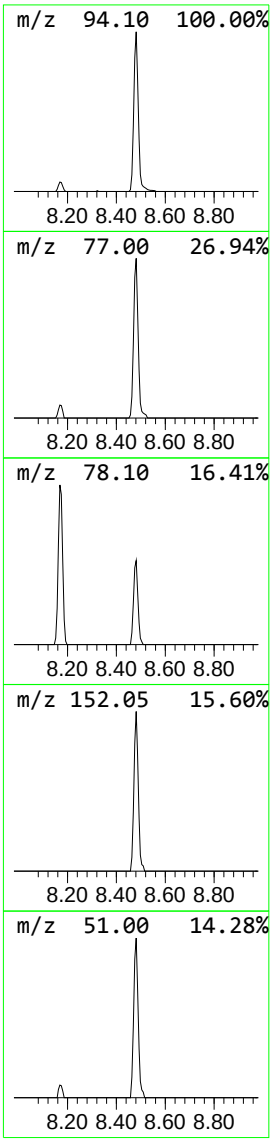
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	4.44 ng	135565	Naphthalene-d8	8.169

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	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59





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BNA_F
ClientSampleId :
UI-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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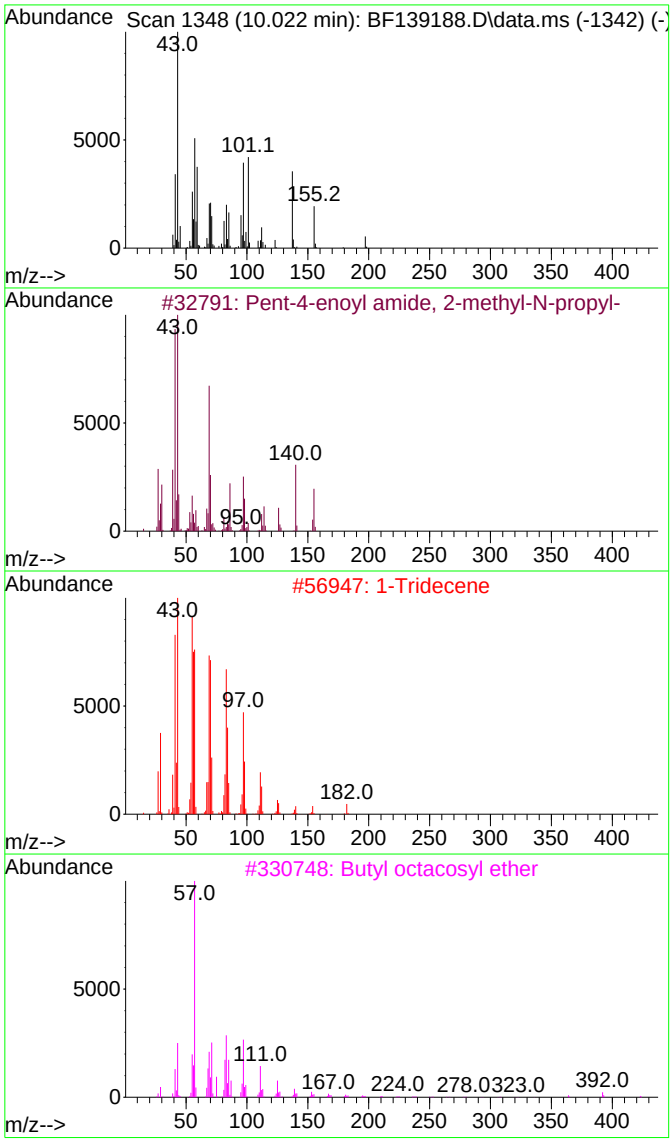
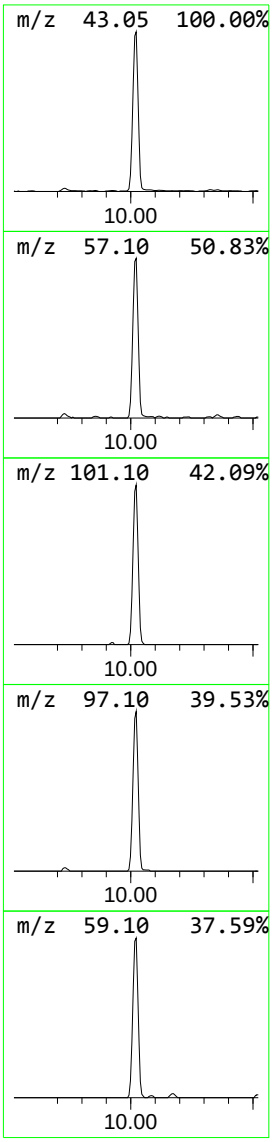
****

Peak Number 6 unknown10.022 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.022	14.76 ng	496435	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	14
2	1-Tridecene	182	C13H26	002437-56-1	14
3	Butyl octacosyl ether	467	C32H66O	1000406-41-1	10
4	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	10
5	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

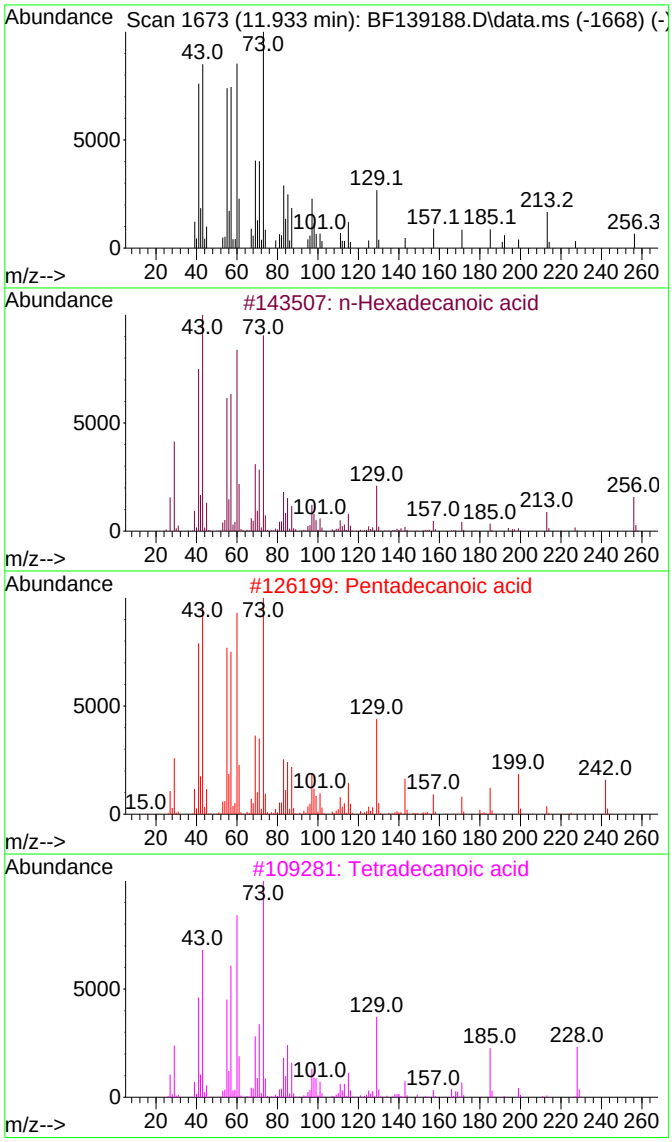
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

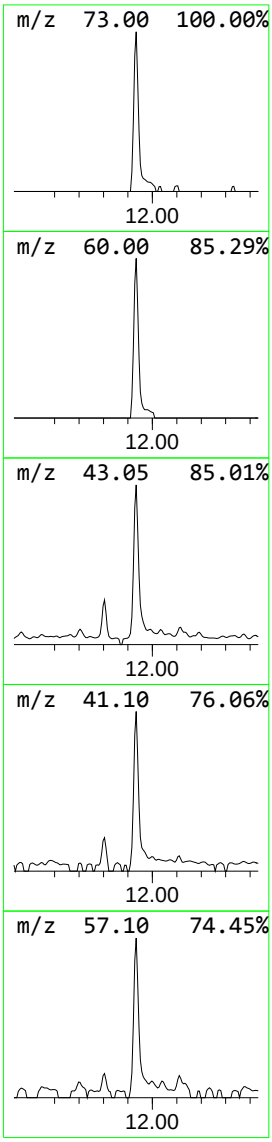
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.934	2.70 ng	82185	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	N-Acetylisoxazolidine	115	C5H9NO2	115615-36-6	25
5	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20





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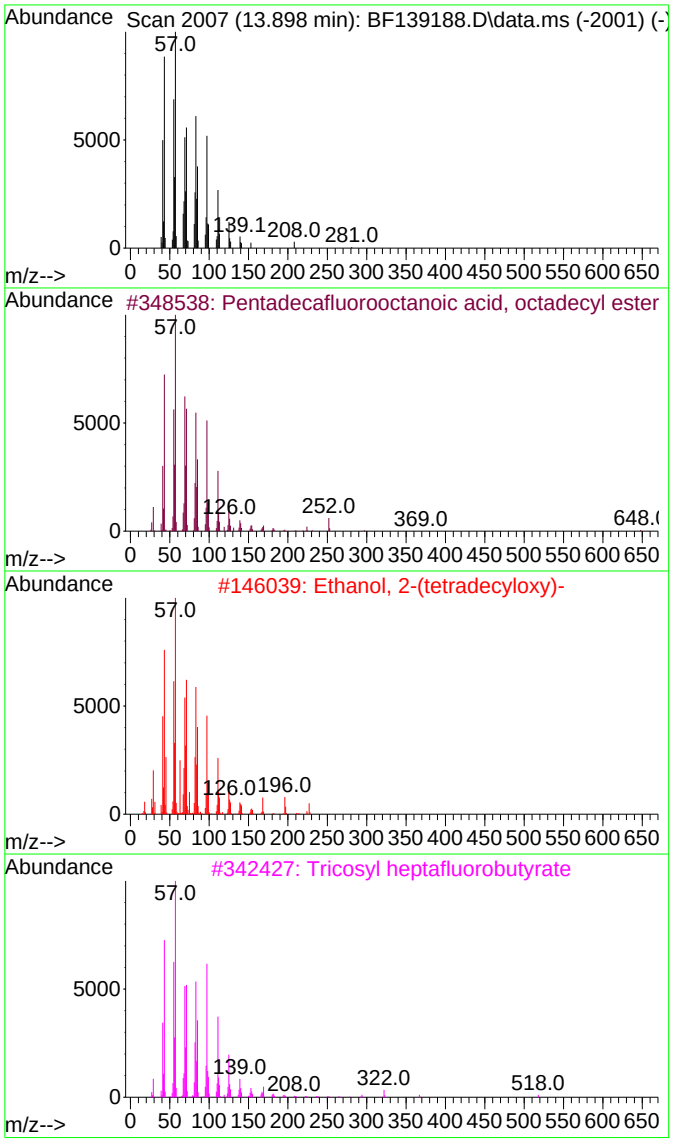
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

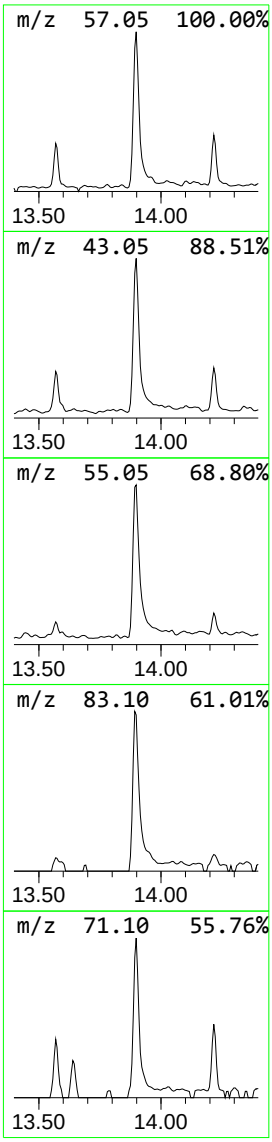
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	5.05 ng	125096	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





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
Butane, 2-metho...	2.187	87.6	ng	2165550	1	6.893	494391	20.0
unknown3.387	3.387	4.2	ng	104254	1	6.893	494391	20.0
2-Pentanone, 4-...	5.110	6.7	ng	165847	1	6.893	494391	20.0
Ethanol, 2-(2-e...	6.710	3.0	ng	73741	1	6.893	494391	20.0
1-Phenoxypropan...	8.481	4.4	ng	135565	2	8.169	610245	20.0
unknown10.022	10.022	14.8	ng	496435	3	9.922	672474	20.0
n-Hexadecanoic ...	11.934	2.7	ng	82185	4	11.410	609700	20.0
Pentadecafluoro...	13.898	5.0	ng	125096	5	14.045	495594	20.0