LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	510	514	526	rVB	327317	422182	18.64%	1.979%
2	5.504	576	581	584	rBV	2231482	2182558	96.37%	10.232%
3	6.510	746	752	757	rBV	2091020	2264858	100.00%	10.618%
4	6.651	771	776	779	rBV	2321158	2248189	99.26%	10.540%
5	6.881	812	815	819	rVB	834453	682796	30.15%	3.201%
6	7.039	838	842	845	rVB	1917990	1631812	72.05%	7.650%
7	7.134	854	858	861	rVB	68515	55174	2.44%	0.259%
8	7.445	905	911	914	rBV	1490687	1385661	61.18%	6.496%
9	8.163	1029	1033	1036	rBV	1091305	889041	39.25%	4.168%
10	8.716	1123	1127	1131	rBV2	27276	31241	1.38%	0.146%
11	8.928	1159	1163	1168	rBV	26863	35959	1.59%	0.169%
12	9.092	1188	1191	1199	rBV2	43403	63120	2.79%	0.296%
13	9.233	1210	1215	1219	rBV	1979522	1926844	85.08%	9.034%
14	9.628	1278	1282	1285	rBV	163962	131138	5.79%	0.615%
15	9.916	1327	1331	1335	rBV2	1067817	933054	41.20%	4.374%
16	10.316	1396	1399	1402	rBV	36947	32923	1.45%	0.154%
17	10.628	1448	1452	1454	rBV	68904	57119	2.52%	0.268%
18	10.704	1461	1465	1474	rVB	1330063	1205881	53.24%	5.654%
19	11.175	1542	1545	1550	rBV	43444	40683	1.80%	0.191%
20	11.404	1580	1584	1587	rBV	928565	804344	35.51%	3.771%
21	11.451	1589	1592	1596	rVB4	22764	22676	1.00%	0.106%
22	11.616	1615	1620	1623	rBV4	16571	23824	1.05%	0.112%
23	11.851	1654	1660	1662	rBV4	19052	24049	1.06%	0.113%
24	11.880	1662	1665	1668	rVV	59644	61933	2.73%	0.290%
25	11.922	1668	1672	1676	rVV	314763	286118	12.63%	1.341%
26	11.957	1676	1678	1681	rVB	57167	43211	1.91%	0.203%
27	12.204	1716	1720	1724	rBV	105064	103704	4.58%	0.486%
28	12.457	1757	1763	1766	rBV	141458	149608	6.61%	0.701%
29	12.627	1787	1792	1797	rBV7	38179	81300	3.59%	0.381%
30	12.704	1802	1805	1812	rBV2	153897	183988	8.12%	0.863%
31	12.863	1827	1832	1838	rBV2	74245	104063	4.59%	0.488%
32	12.916	1838	1841	1844	rVV	71540	60180	2.66%	0.282%
33	12.986	1849	1853	1856	rVB	1296549	1157867	51.12%	5.428%
34	13.392	1919	1922	1926	rBV6	19486	35842	1.58%	0.168%

LSC Area Percent Report

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Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

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:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.457	1930	1933	1935	rVV	91025	73393	3.24%	0.344%
36	13.657	1964	1967	1973	rBV4	75154	104953	4.63%	0.492%
37	13.839	1996	1998	2000	rVB	30397	23944	1.06%	0.112%
38	13.868	2000	2003	2007	rBV	118814	118450	5.23%	0.555%
39	14.010	2024	2027	2029	rBV	192264	163171	7.20%	0.765%
40	14.039	2029	2032	2036	rVB	794207	681037	30.07%	3.193%
41	14.168	2051	2054	2057	rBV	54517	54444	2.40%	0.255%
42	14.210	2058	2061	2063	rVB	75672	70229	3.10%	0.329%
43	15.515	2278	2283	2291	rVB	509386	677181	29.90%	3.175%

Sum of corrected areas: 21329742

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
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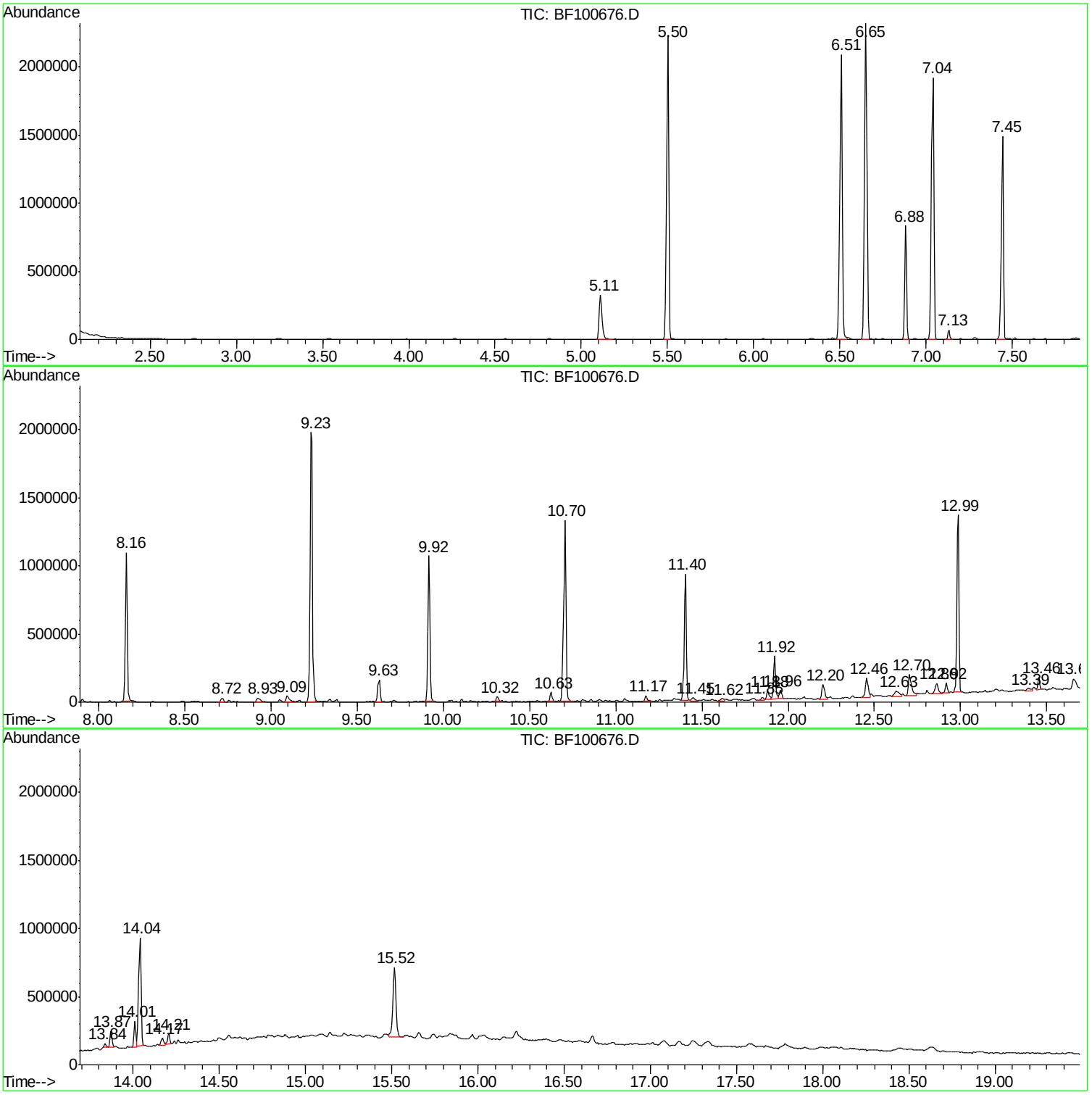
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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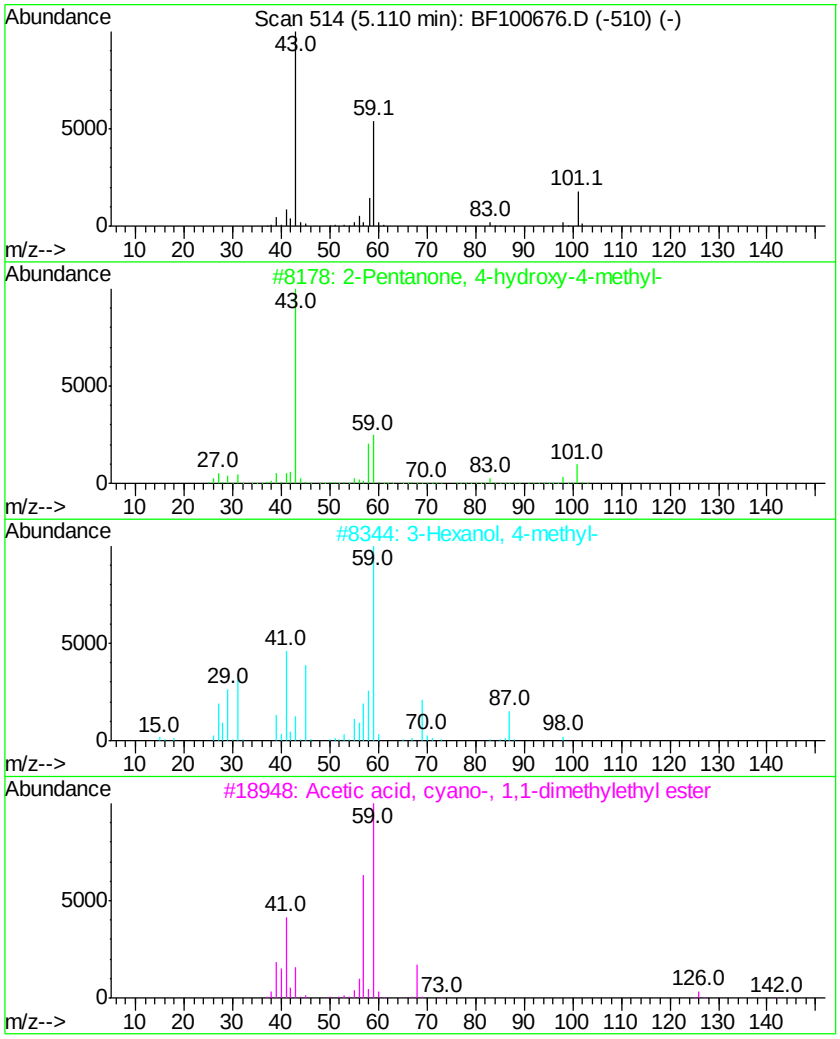
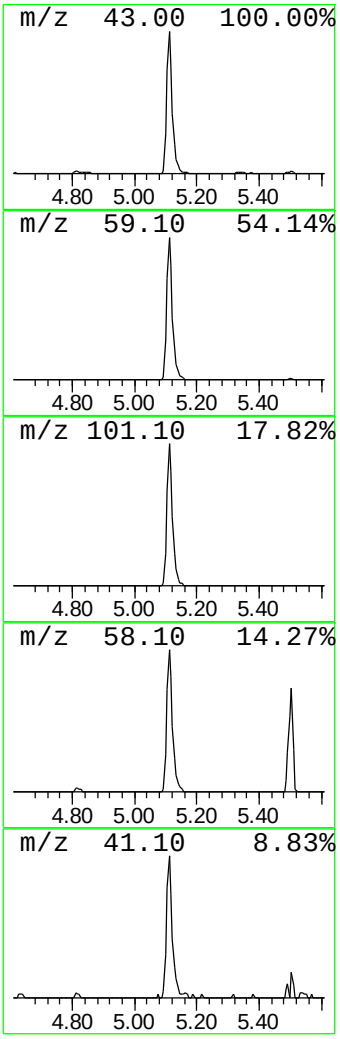
Peak Number 1 unknown5.11 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	12.37 ng	422182	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

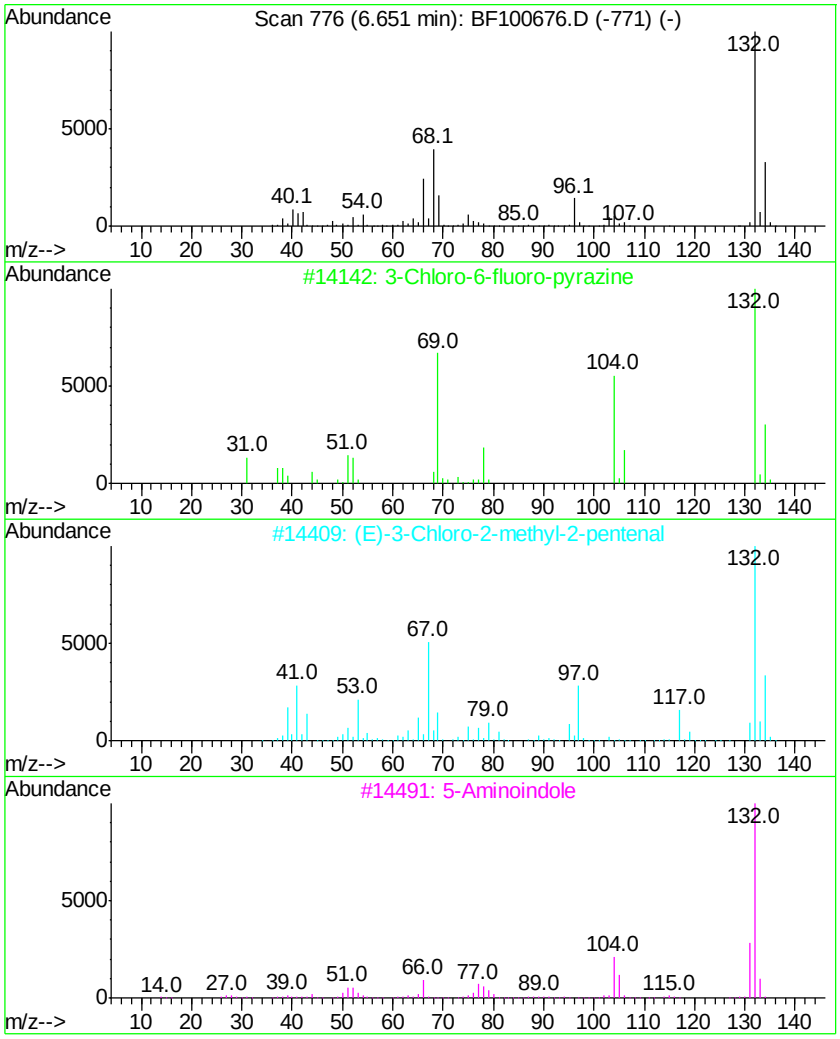
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

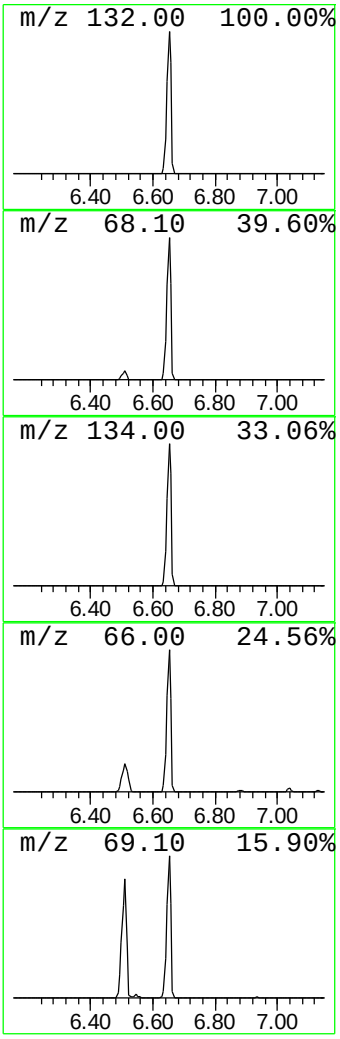
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	65.85 ng	2248190	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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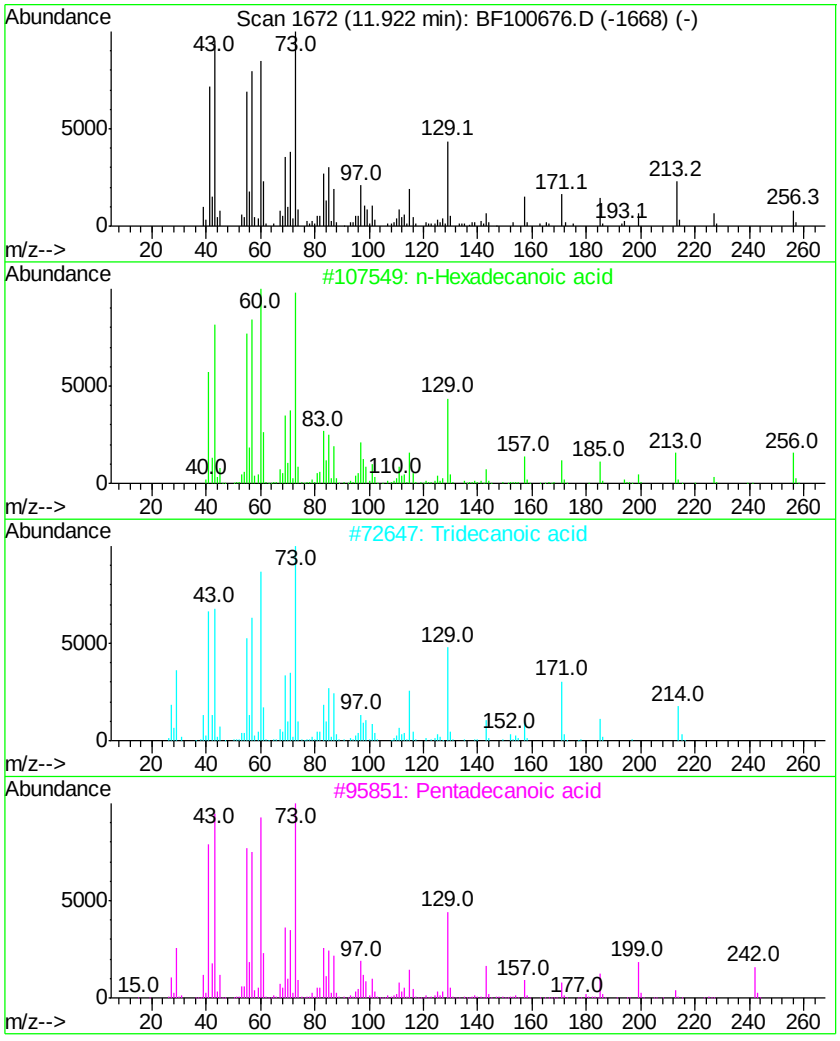
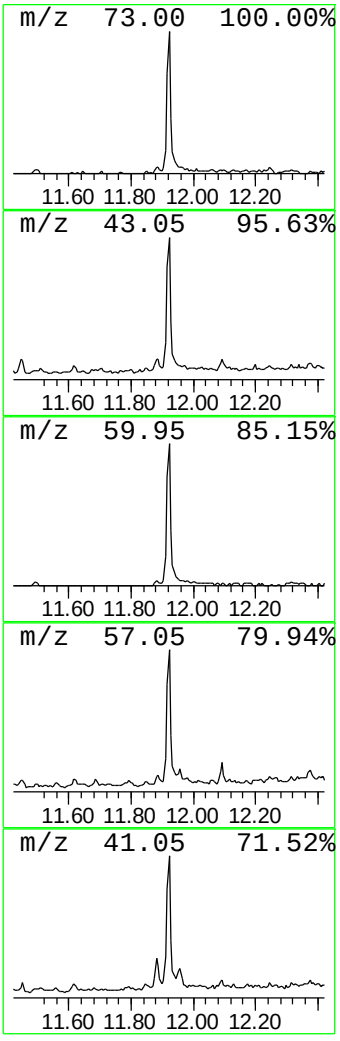
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	7.11 ng	286118	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

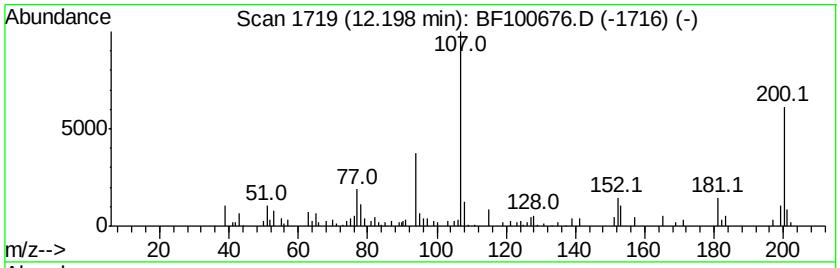
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

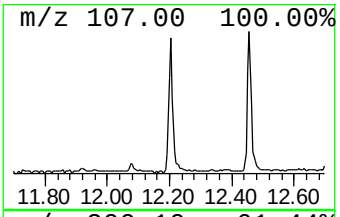
****

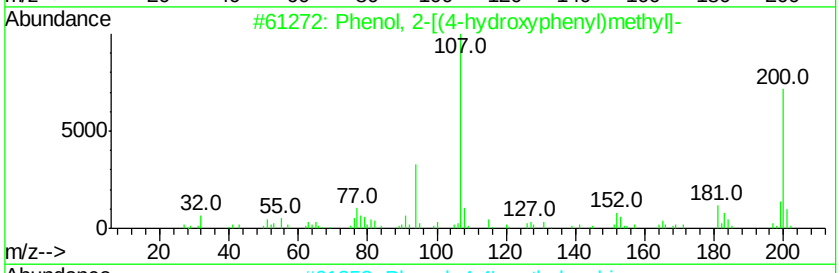
Peak Number 5 Phenol, 2-[(4-hydroxyphenyl... Concentration Rank 10

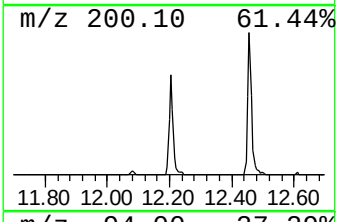
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.20	2.58 ng	103704	Phenanthrene-d10	11.40

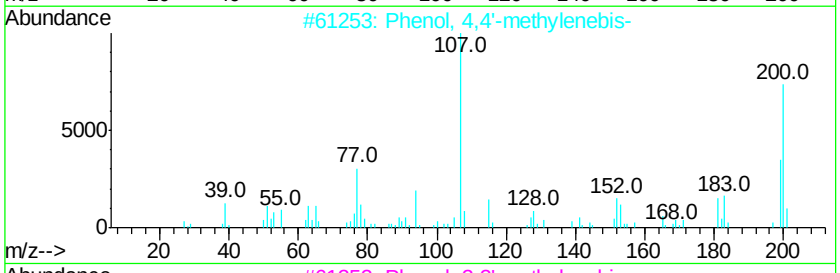
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	94
2	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	91
3	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	91
4	Benzenepropanoic acid, .alpha.,4...	182	C9H10O4	000306-23-0	38
5	4-(2-Methoxyethyl)phenol	152	C9H12O2	056718-71-9	38

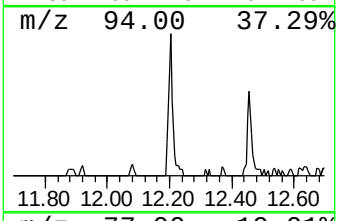


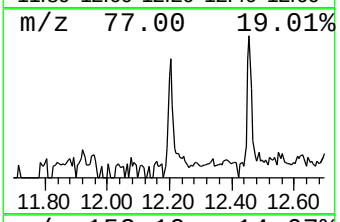


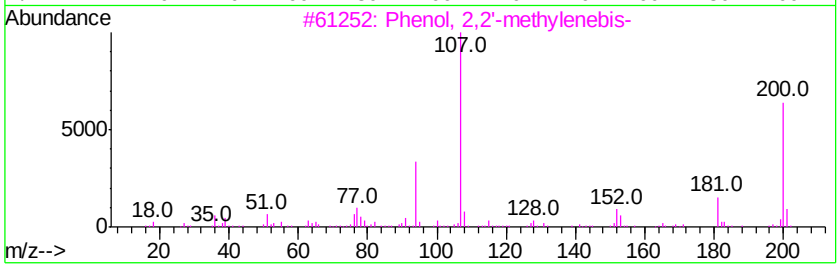


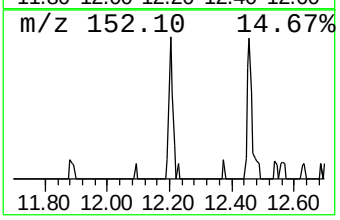












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Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

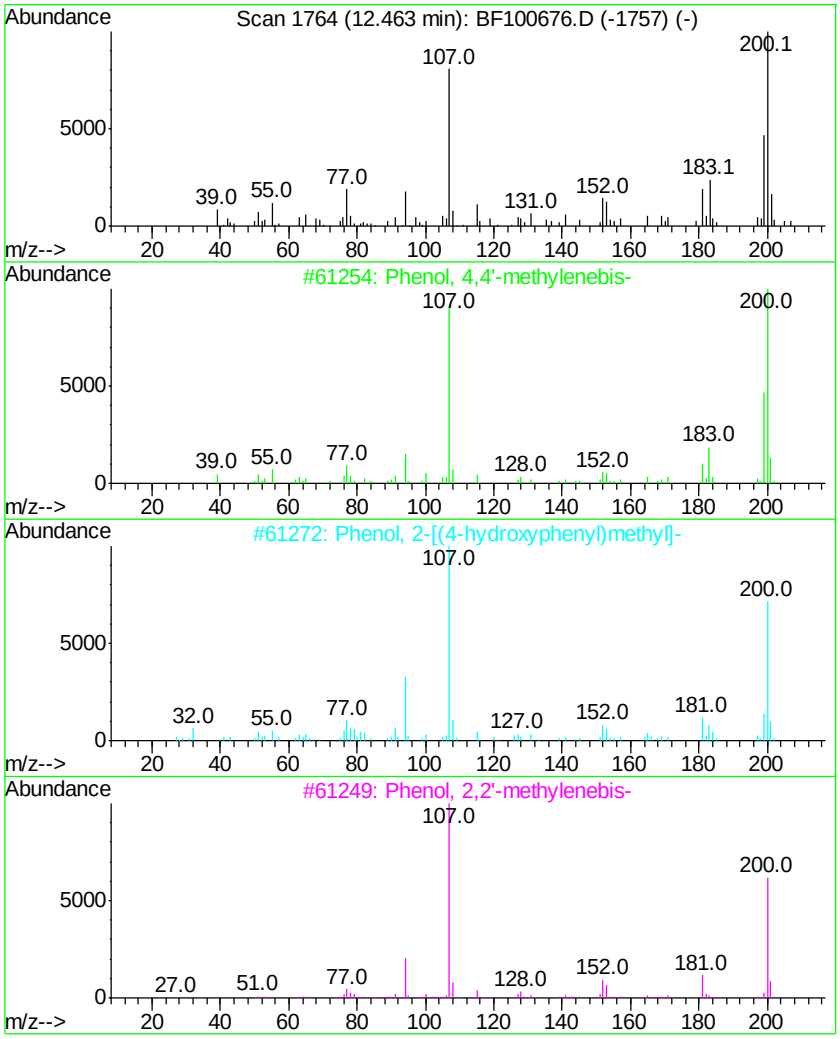
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

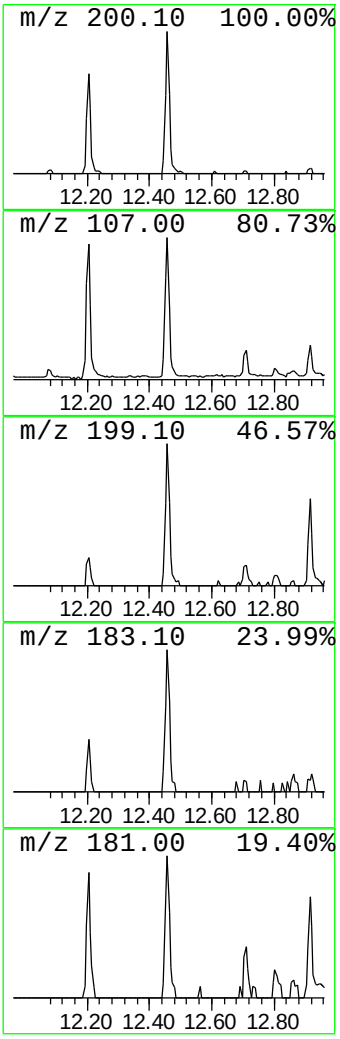
****

Peak Number 6 Phenol, 4,4'-methylenebis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	3.72 ng	149608	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	95
2	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	94
3	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	81
4	1,3-Benzenediol, 4-(phenylmethyl)-	200	C13H12O2	002284-30-2	64
5	2-Stilbazole, 4'-hydroxydihydro-	199	C13H13NO	085666-07-5	43





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Misc :
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Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

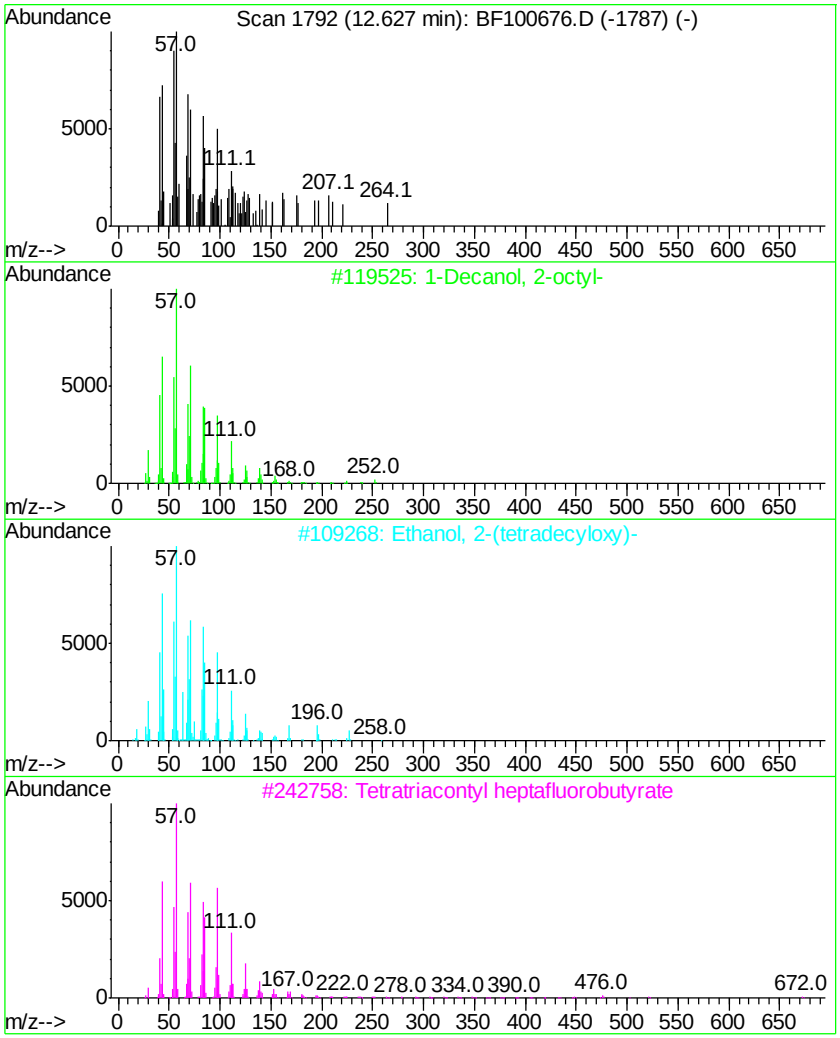
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

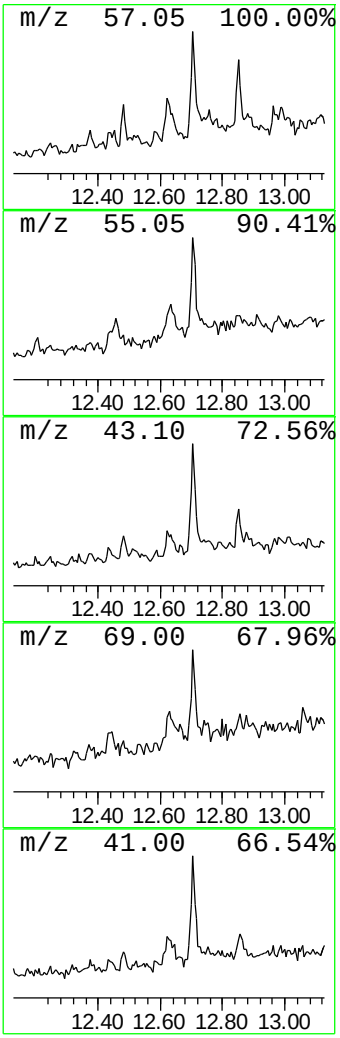
****

Peak Number 7 1-Decanol, 2-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	2.02 ng	81300	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	72
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	72
3	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	64
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	64
5	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
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Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

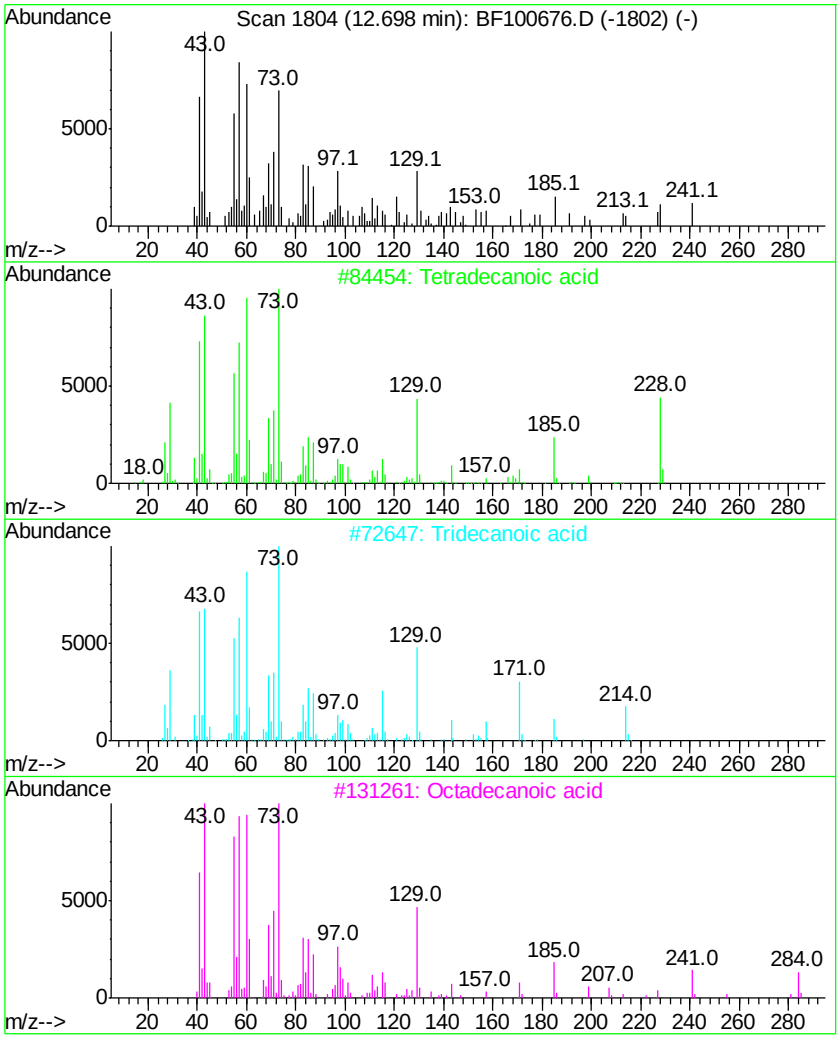
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

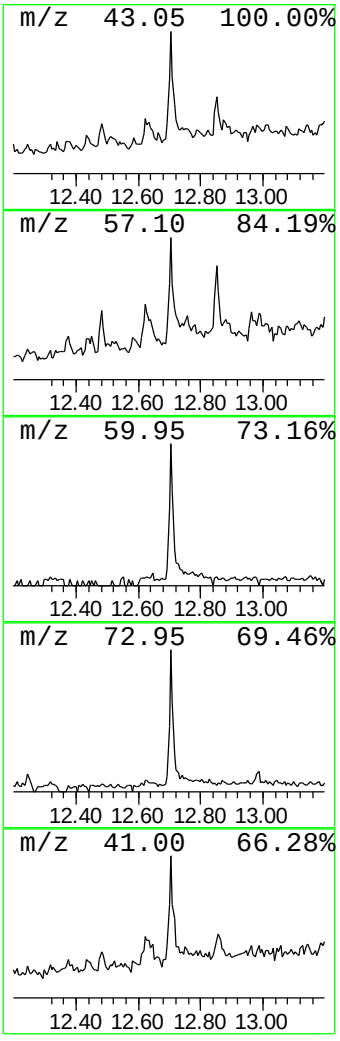
****

Peak Number 8 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.57 ng	183988	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Octadecanoic acid	284	C18H36O2	000057-11-4	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111717\
Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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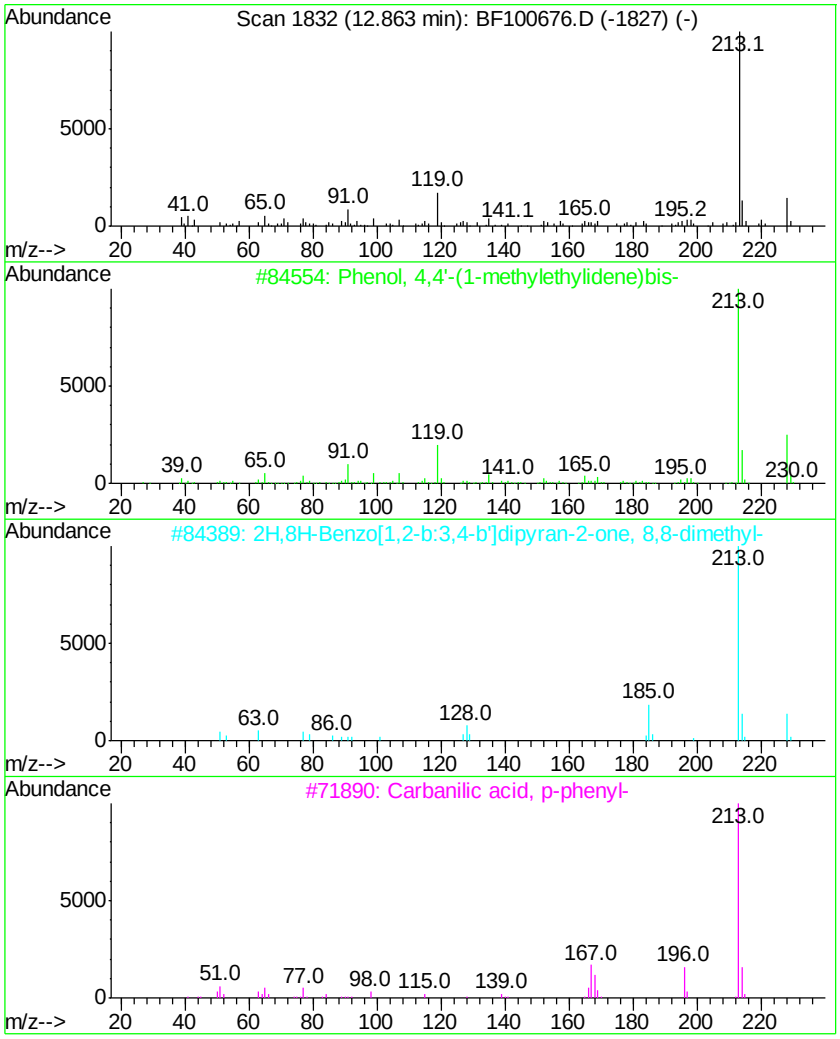
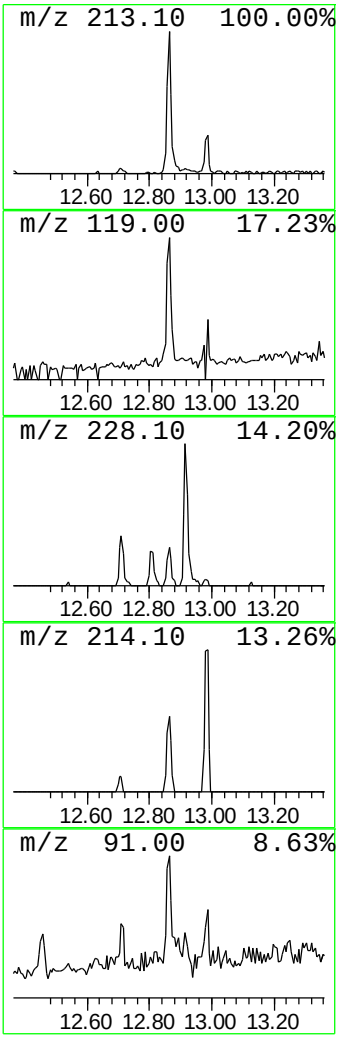
Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	3.06 ng	104063	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	64
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	64
4	1,4-Naphthalenedione, 2-(1-buten...	228	C14H12O3	029366-43-6	53
5	Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	53





Library Search Compound Report

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Data File : BF100676.D
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Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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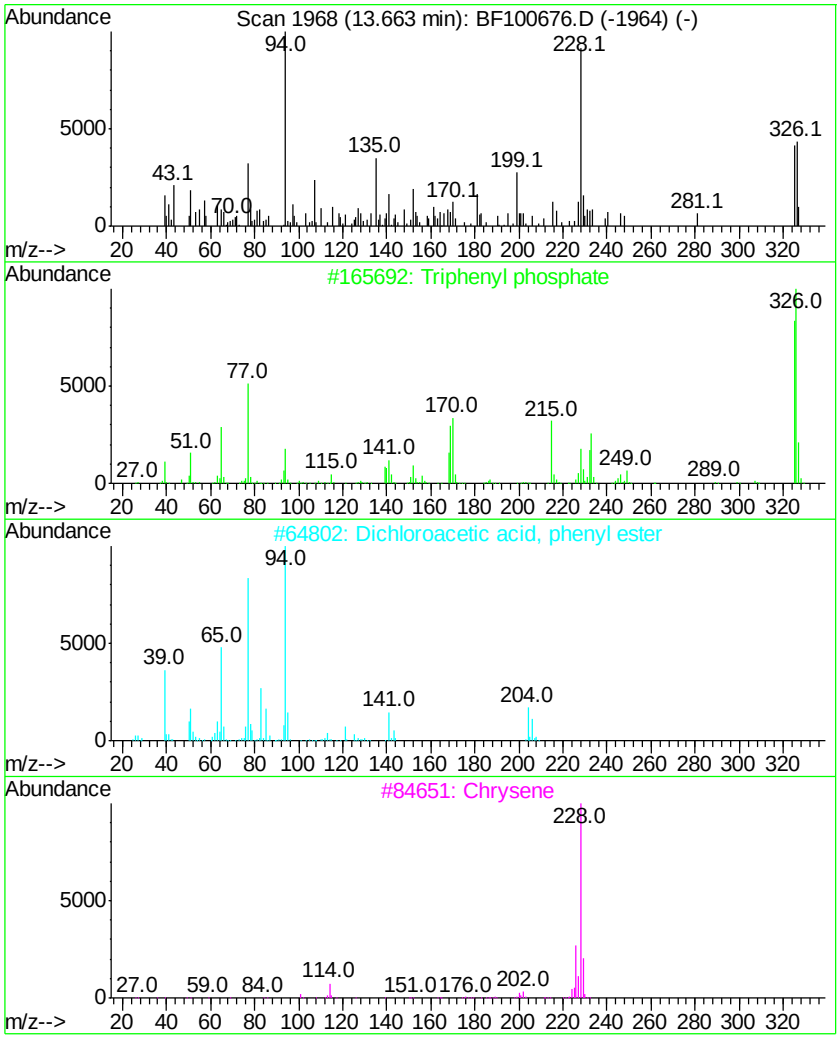
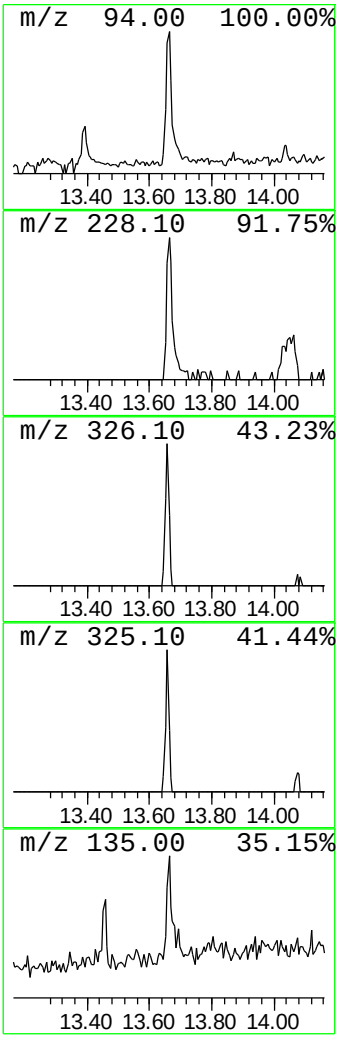
Peak Number 10 Triphenyl phosphate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	3.08 ng	104953	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenyl phosphate	326	C18H15O4P	000115-86-6	98
2	Dichloroacetic acid, phenyl ester	204	C8H6Cl2O2	010565-20-5	32
3	Chrysene	228	C18H12	000218-01-9	11
4	Methyl-3-phenoxybenzoate	228	C14H12O3	050789-43-0	11
5	Benzene, (ethylsulfonyl)-	170	C8H10O2S	000599-70-2	10





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Data File : BF100676.D
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Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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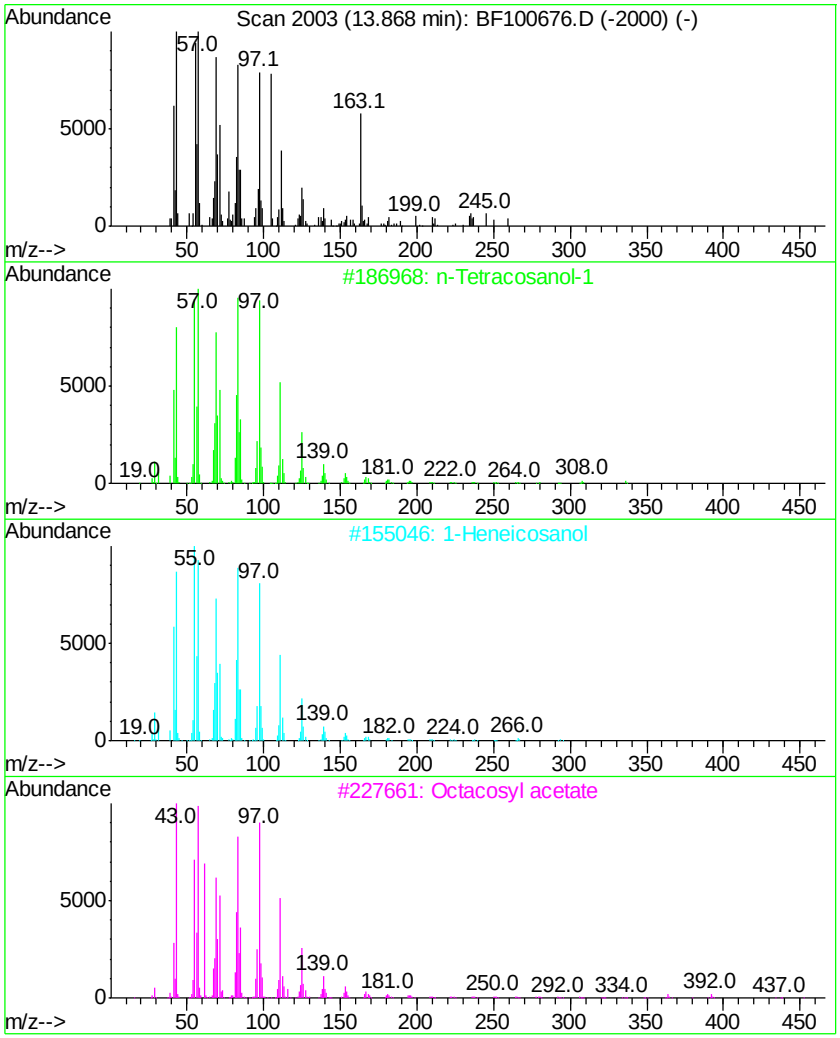
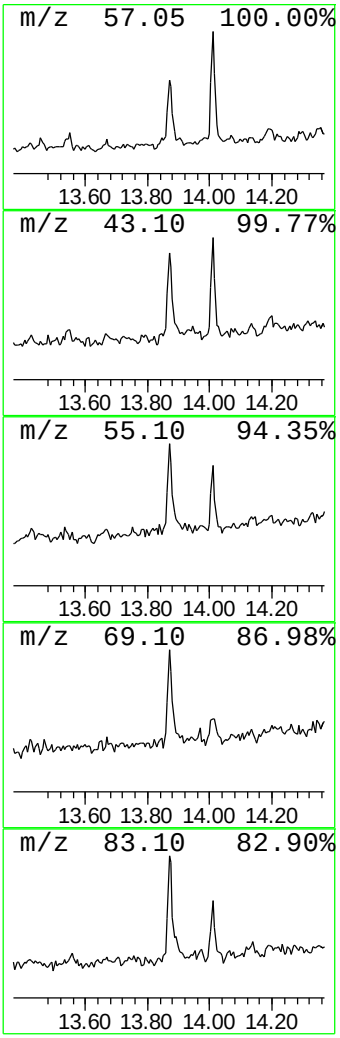
Peak Number 11 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	3.48 ng	118450	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Octacosyl acetate	452	C30H60O2	018206-97-8	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5	Cyclopentadecane	210	C15H30	000295-48-7	87





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Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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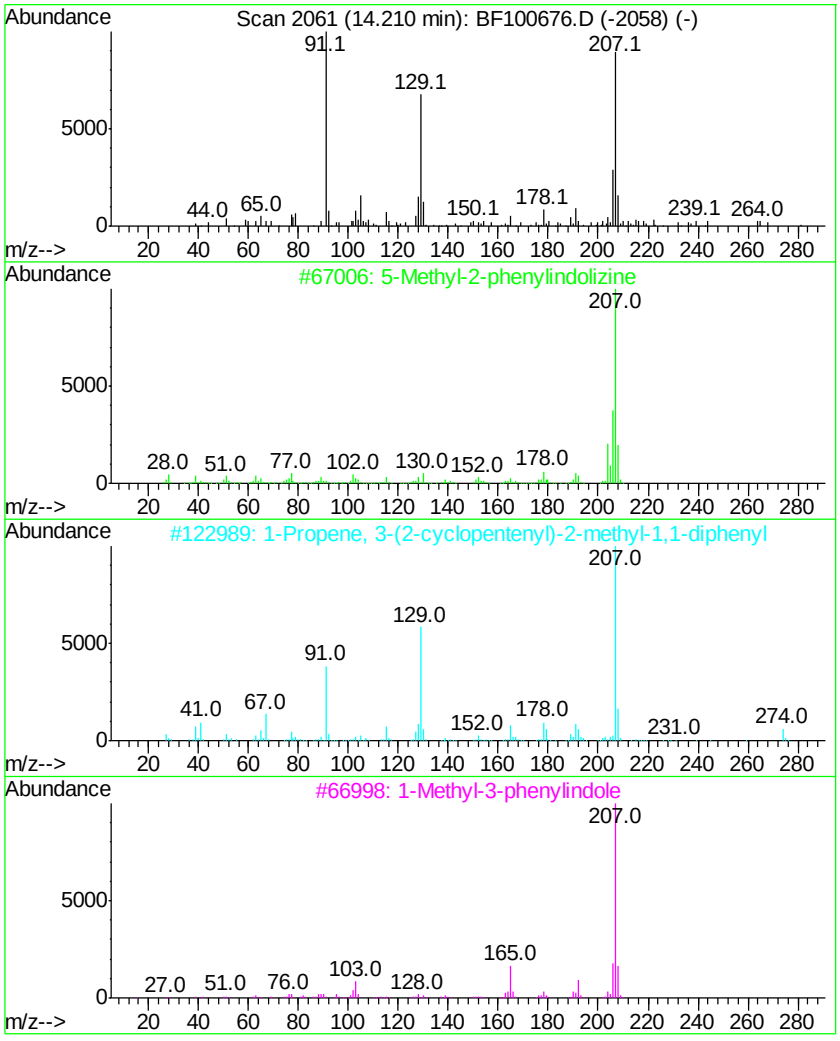
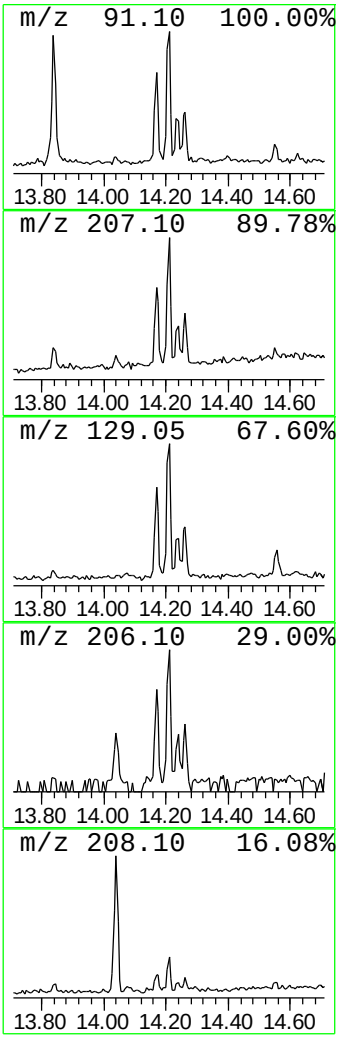
Peak Number 12 unknown14.21 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	2.06 ng	70229	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	47
2	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	45
3	1-Methyl-3-phenylindole	207	C15H13N	030020-98-5	38
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	38





Tentatively Identified Compound (LSC) summary

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Data File : BF100676.D
Acq On : 17 Nov 2017 15:18
Operator : SJ/JU
Sample : I6454-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-GURABO-S001-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.11	5.11	12.4	ng	422182	1	6.88	682796	20.0
unknown6.65	6.65	65.8	ng	2248190	1	6.88	682796	20.0
n-Hexadecanoic acid	11.92	7.1	ng	286118	4	11.40	804344	20.0
Phenol, 2-[(4-hyd...	12.20	2.6	ng	103704	4	11.40	804344	20.0
Phenol, 4,4'-meth...	12.46	3.7	ng	149608	4	11.40	804344	20.0
1-Decanol, 2-octyl-	12.63	2.0	ng	81300	4	11.40	804344	20.0
Tetradecanoic acid	12.70	4.6	ng	183988	4	11.40	804344	20.0
Phenol, 4,4'-(1-m...	12.86	3.1	ng	104063	5	14.04	681037	20.0
Triphenyl phosphate	13.66	3.1	ng	104953	5	14.04	681037	20.0
n-Tetracosanol-1	13.87	3.5	ng	118450	5	14.04	681037	20.0
unknown14.21	14.21	2.1	ng	70229	5	14.04	681037	20.0