LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
Data File : BF134139.D
Acq On : 07 Jul 2023 15:50
Operator : CG\JU
Sample : 03392-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SRY-1

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: BF134139.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	18	rVB	1219005	1578999	66.05%	8.354%
2	2.252	24	28	37	rVB	46277	64138	2.68%	0.339%
3	5.093	506	511	520	rBV	66767	91296	3.82%	0.483%
4	5.481	573	577	586	rBV	2334655	2194837	91.80%	11.612%
5	6.487	743	748	767	rVB	2002588	2208036	92.36%	11.681%
6	6.846	805	809	817	rBV	829329	682660	28.55%	3.612%
7	7.410	900	905	908	rBV	1514109	1373167	57.44%	7.265%
8	8.122	1023	1026	1030	rBV	977869	811406	33.94%	4.293%
9	9.204	1206	1210	1213	rBV	2833327	2390783	100.00%	12.648%
10	9.351	1232	1235	1238	rVB	33919	28727	1.20%	0.152%
11	9.739	1299	1301	1304	rVB	29551	27430	1.15%	0.145%
12	9.881	1322	1325	1329	rBV	933917	773172	32.34%	4.090%
13	10.304	1391	1397	1402	rBV4	27891	51958	2.17%	0.275%
14	10.398	1410	1413	1417	rBV	74417	63856	2.67%	0.338%
15	10.598	1442	1447	1454	rBV	208543	189944	7.94%	1.005%
16	10.675	1456	1460	1465	rBV	1389264	1230845	51.48%	6.512%
17	10.798	1477	1481	1486	rVB3	22262	35229	1.47%	0.186%
18	10.981	1509	1512	1516	rBV2	55947	51088	2.14%	0.270%
19	11.375	1576	1579	1582	rBV	724013	622816	26.05%	3.295%
20	11.404	1582	1584	1586	rVB	36273	29060	1.22%	0.154%
21	11.486	1595	1598	1601	rBV4	26524	28215	1.18%	0.149%
22	11.910	1666	1670	1674	rBV	438857	437293	18.29%	2.313%
23	12.204	1717	1720	1724	rBV3	69136	83055	3.47%	0.439%
24	12.457	1761	1763	1768	rBV2	76520	99187	4.15%	0.525%
25	12.598	1784	1787	1789	rBV	205415	175068	7.32%	0.926%
26	12.704	1802	1805	1812	rBV3	166611	217591	9.10%	1.151%
27	12.792	1818	1820	1822	rBV	61040	49473	2.07%	0.262%
28	12.827	1824	1826	1832	rVB	164267	163743	6.85%	0.866%
29	12.975	1845	1851	1855	rBV	1983229	1864888	78.00%	9.866%
30	13.175	1883	1885	1888	rVB4	112793	92504	3.87%	0.489%
31	14.039	2028	2032	2035	rBV2	625673	667620	27.92%	3.532%
32	15.551	2285	2289	2297	rVB	340226	524133	21.92%	2.773%

Sum of corrected areas: 18902217

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Operator : CG\JU
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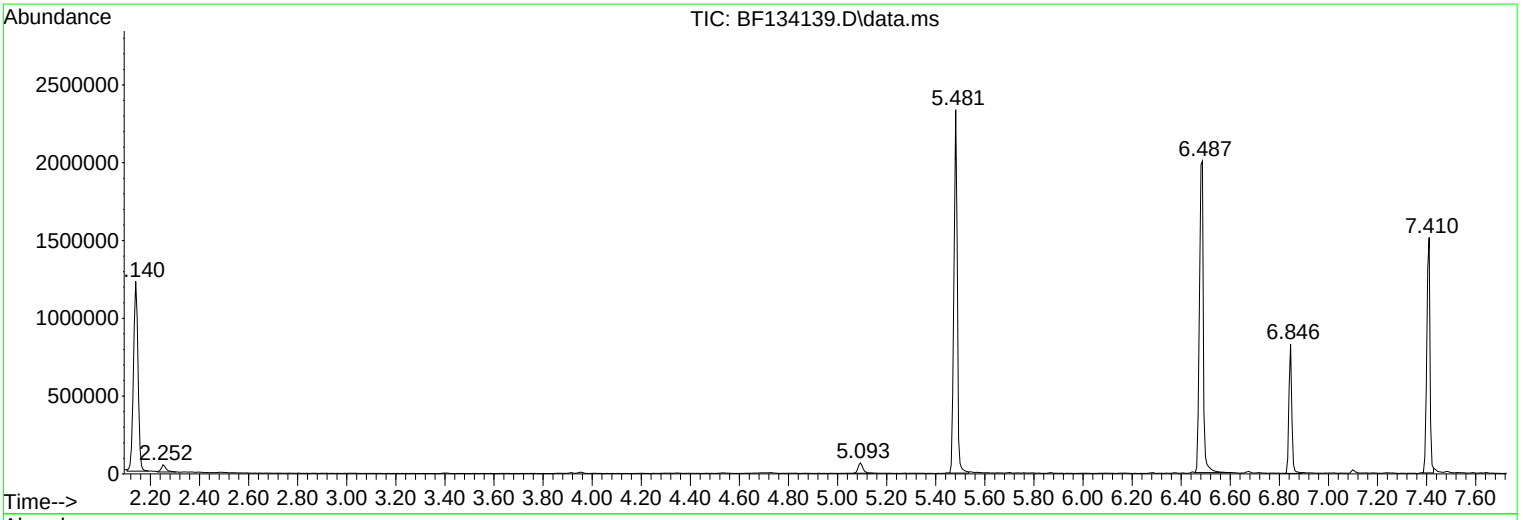
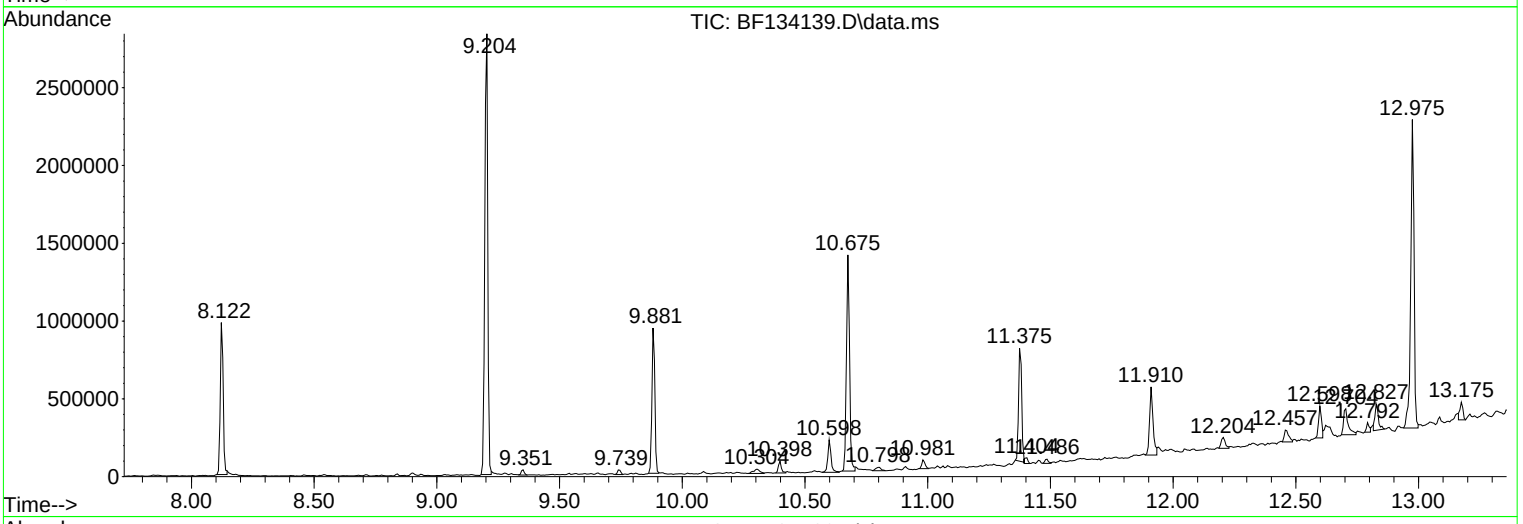
Misc :
ALS Vial : 36 Sample Multiplier: 1

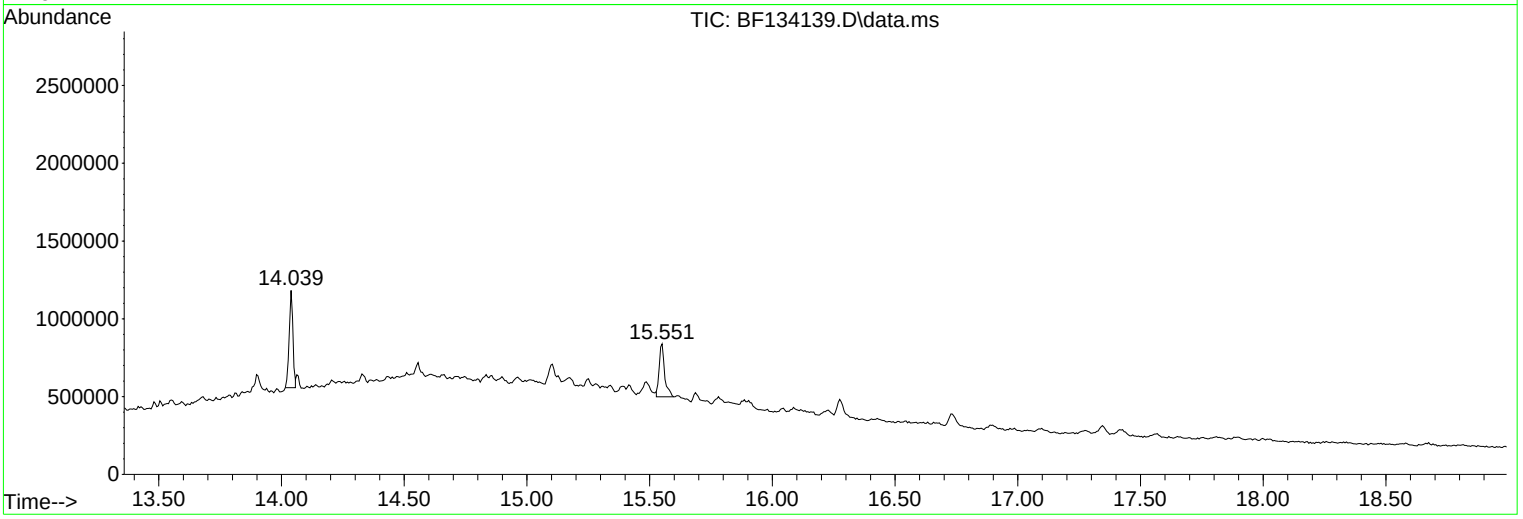
Instrument :
BNA_F
ClientSampleId :
SRY-1

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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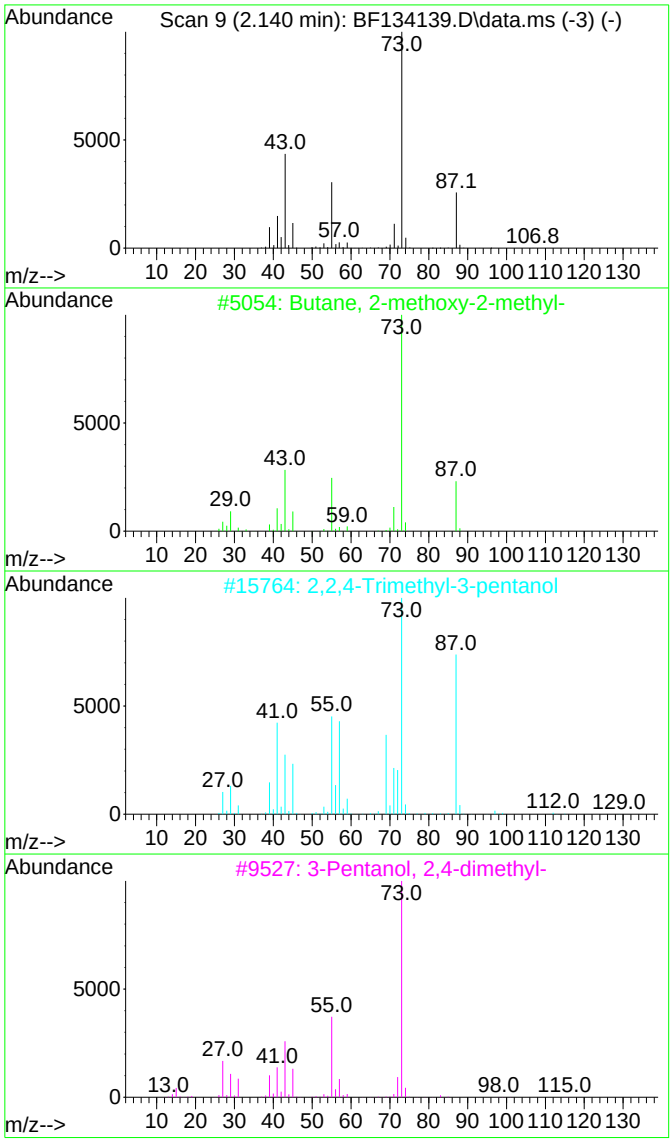
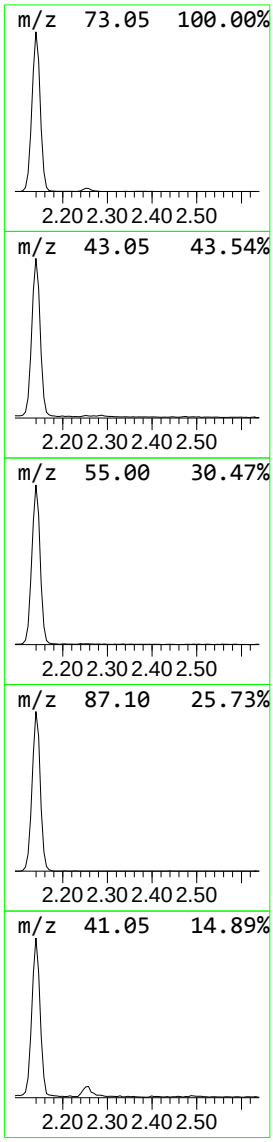
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	46.26 ng	1579000	1,4-Dichlorobenzene-d4	6.846

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Instrument :
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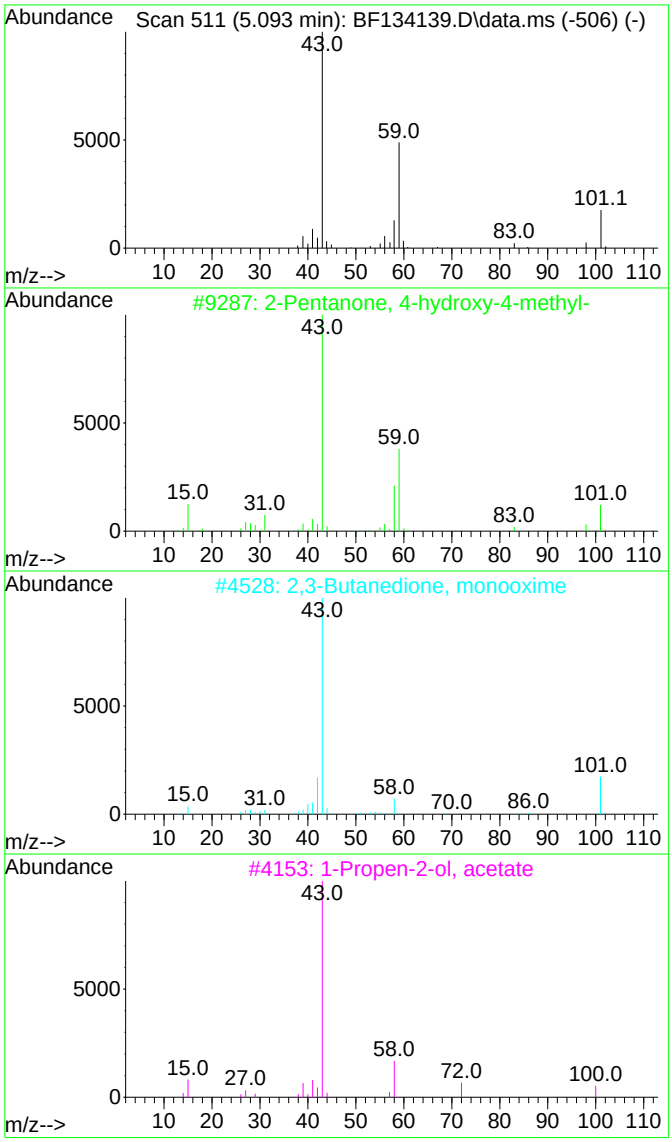
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

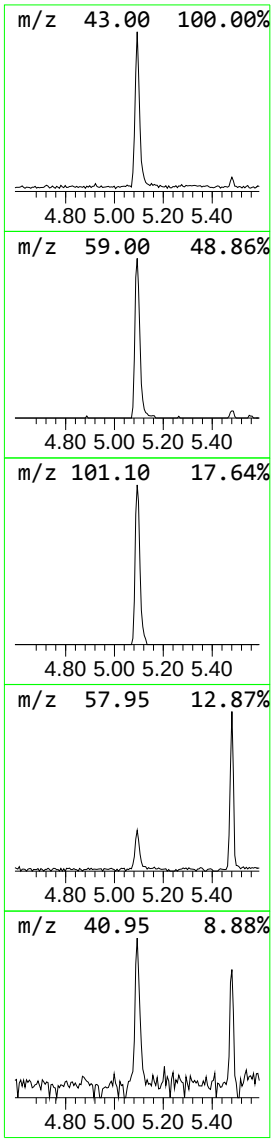
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.67 ng	91296	1,4-Dichlorobenzene-d4	6.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9





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

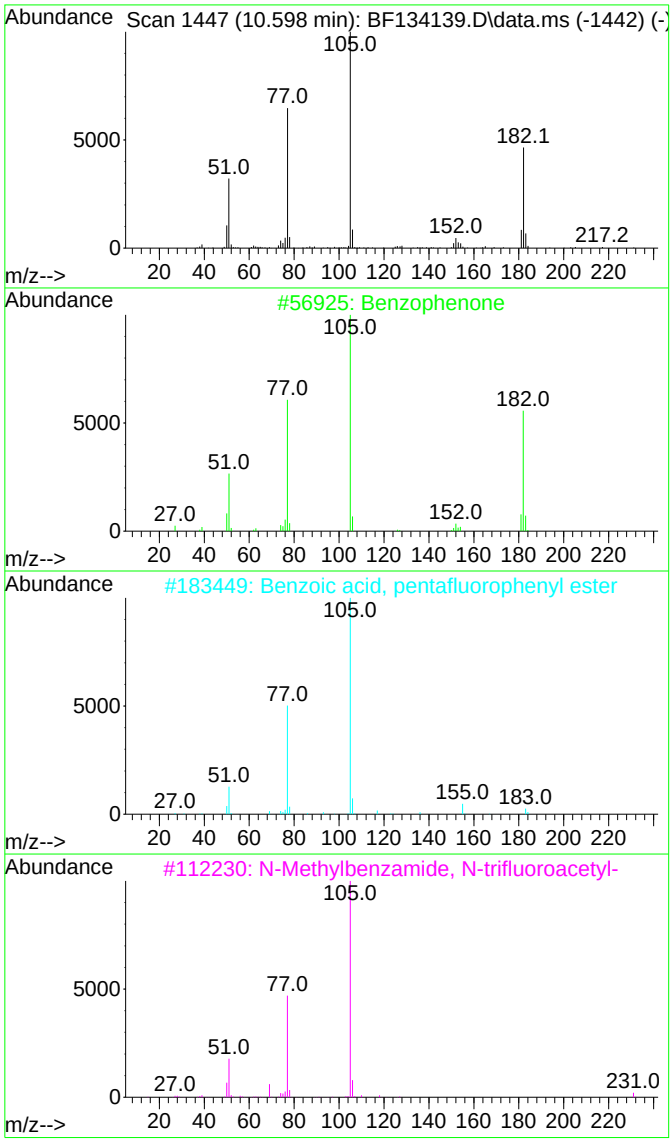
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

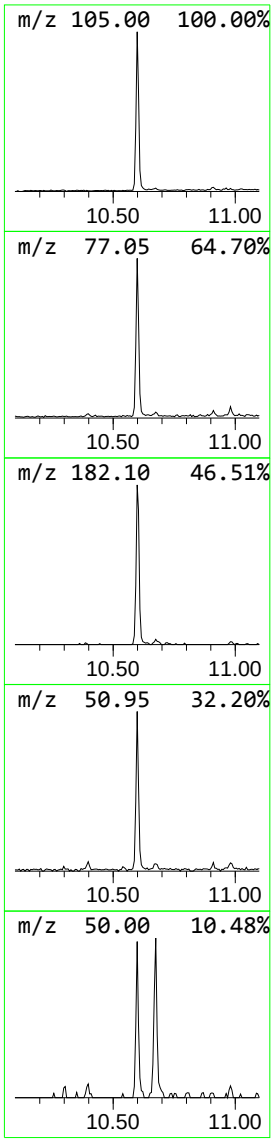
****

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.598	4.91 ng	189944	Acenaphthene-d10	9.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
3	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	49
4	Ethanone, 2,2-dihydroxy-1-phenyl-	152	C8H8O3	001075-06-5	47
5	Benzoylformic acid	150	C8H6O3	000611-73-4	47





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

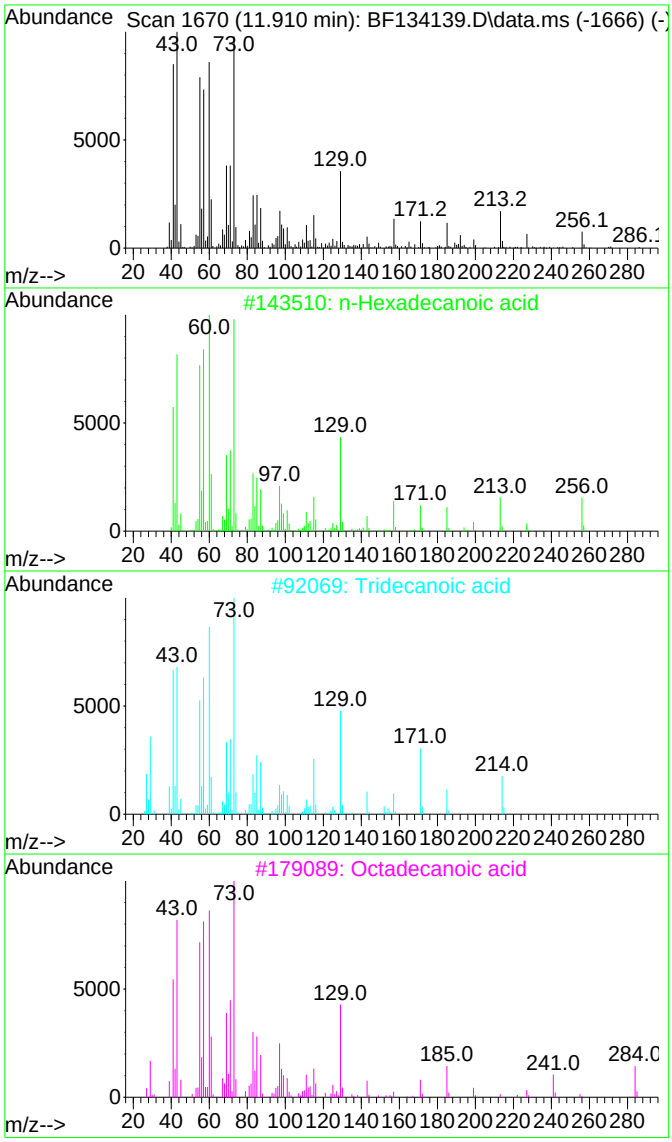
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

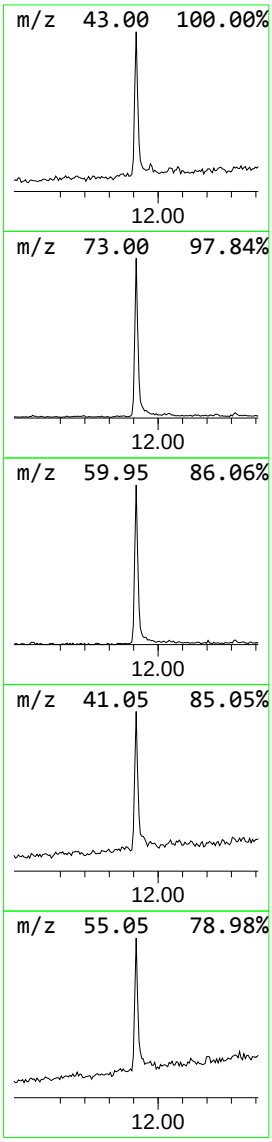
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	14.04 ng	437293	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	86





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ALS Vial : 36 Sample Multiplier: 1

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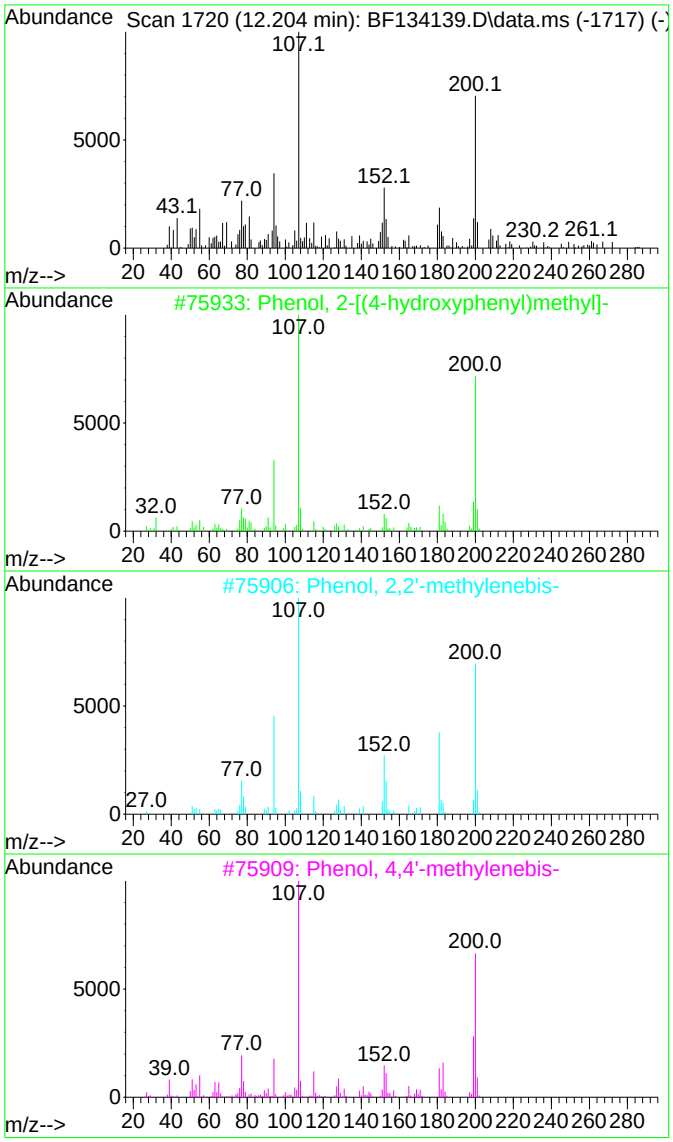
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

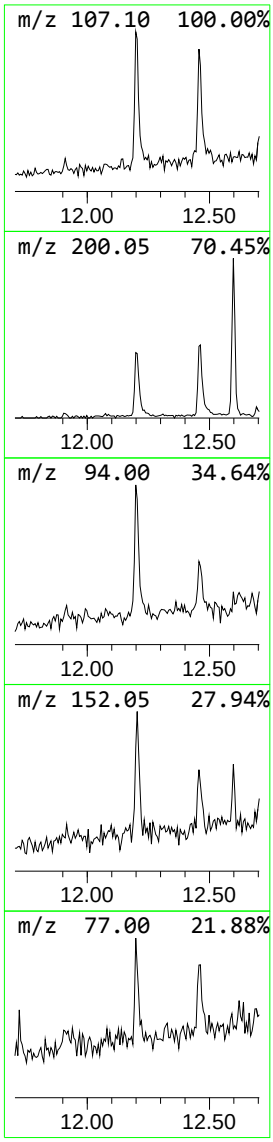
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 2-[(4-hydroxyphenyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.204	2.67 ng	83055	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	87
2	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	76
3	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	68
4	2,2'-Methylenediphenol, diacetate	284	C17H16O4	038782-65-9	64
5	Benzeneacetic acid, 4-hydroxy-	152	C8H8O3	000156-38-7	38





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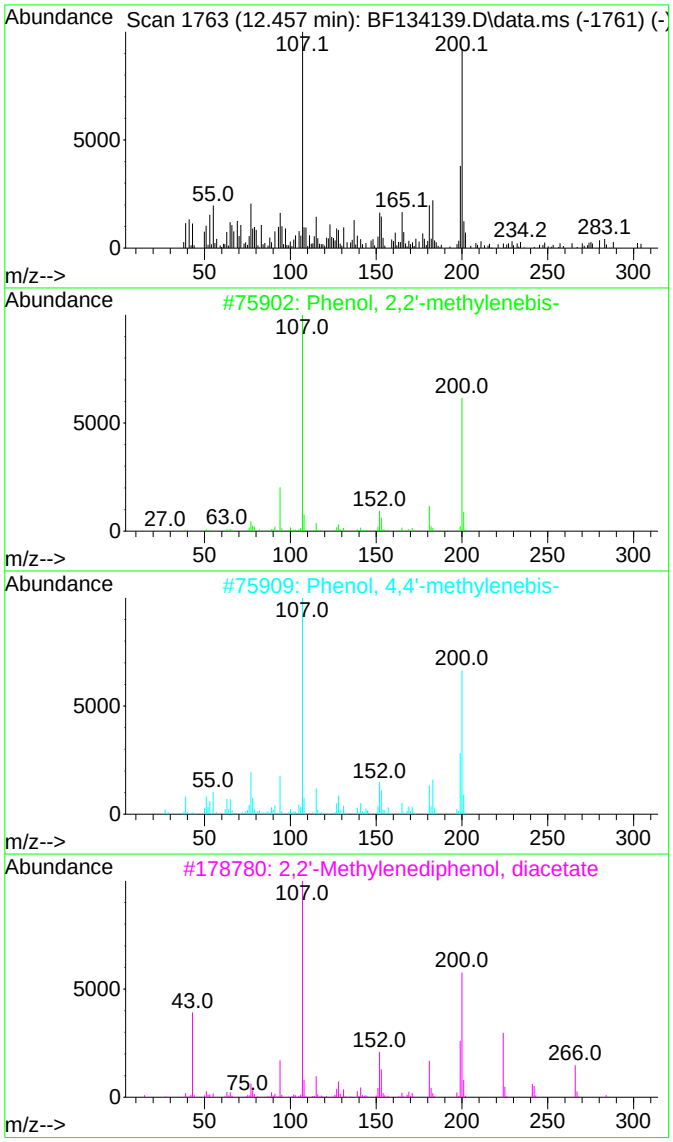
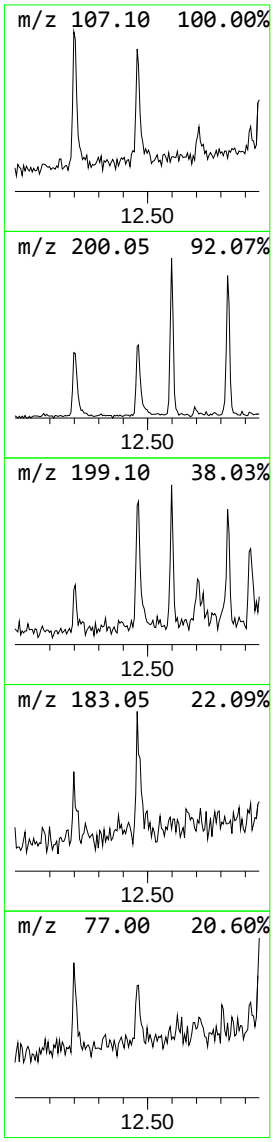
****

Peak Number 6 Phenol, 2,2'-methylenebis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	3.19 ng	99187	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,2'-methylenebis-	200	C13H12O2	002467-02-9	95
2	Phenol, 4,4'-methylenebis-	200	C13H12O2	000620-92-8	94
3	2,2'-Methylenediphenol, diacetate	284	C17H16O4	038782-65-9	83
4	Phenol, 2-[(4-hydroxyphenyl)meth...	200	C13H12O2	002467-03-0	81
5	1,3-Benzenediol, 4-(phenylmethyl)-	200	C13H12O2	002284-30-2	50





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Instrument :
BNA_F
ClientSampleId :
SRY-1

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

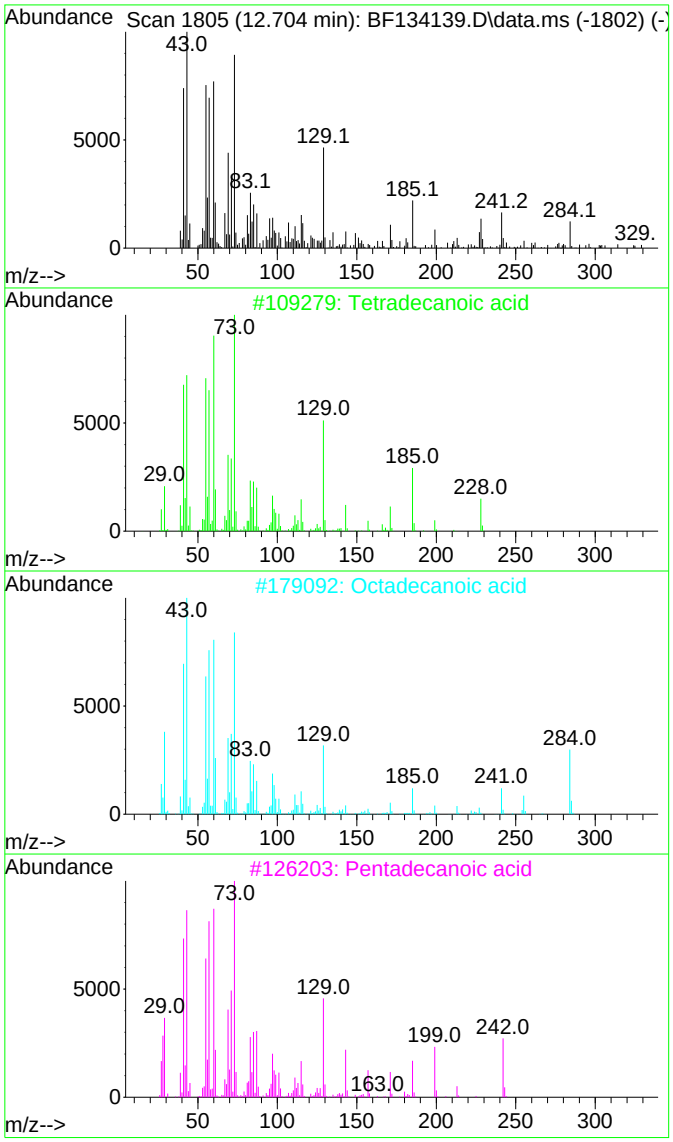
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

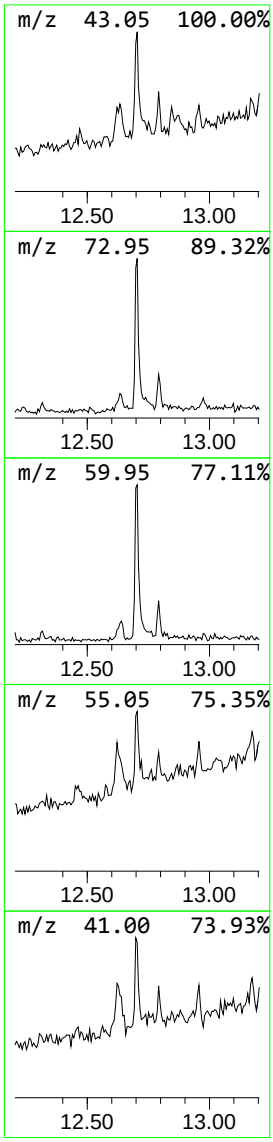
****

Peak Number 7 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	6.99 ng	217591	Phenanthrene-d10	11.375

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
2	Octadecanoic acid	284	C18H36O2	000057-11-4	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	83
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70





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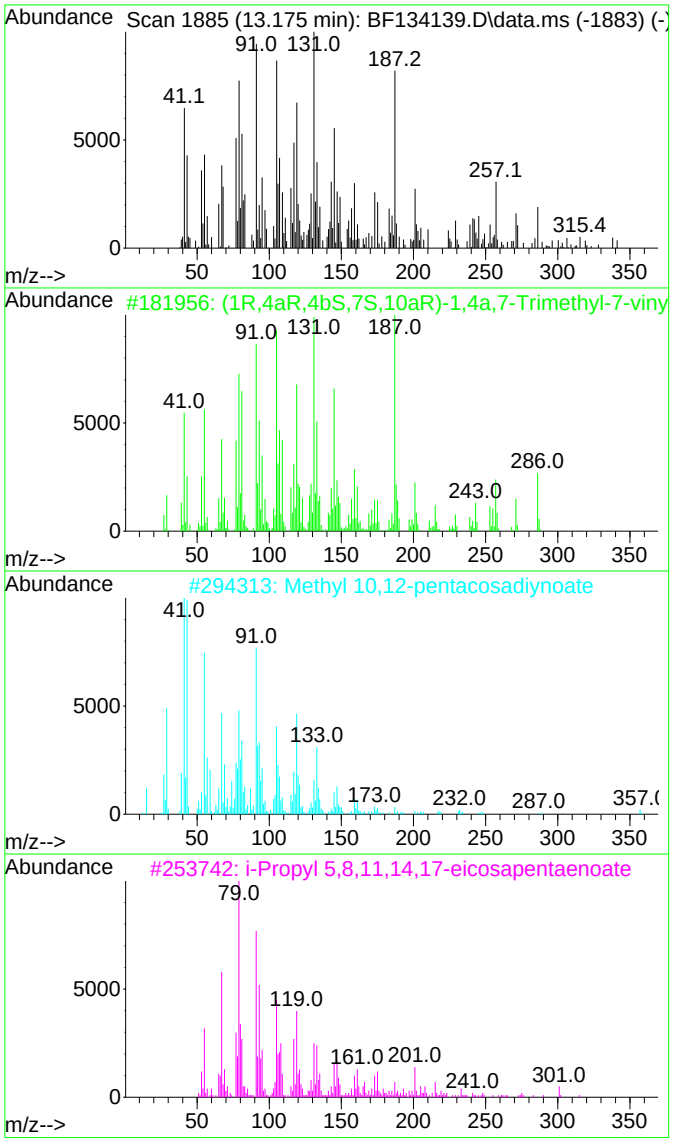
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

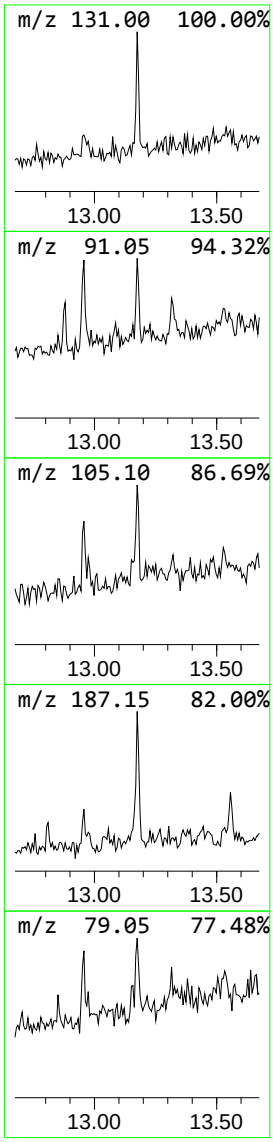
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (1R,4aR,4bS,7S,10aR)-1,4a,7... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.175	2.77 ng	92504	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,4aR,4bS,7S,10aR)-1,4a,7-Trim...	286	C20H30O	001686-63-1	68
2	Methyl 10,12-pentacosadiynoate	388	C26H44O2	1000342-58-7	35
3	i-Propyl 5,8,11,14,17-eicosapent...	344	C23H36O2	1000336-72-2	27
4	4,5-Diphenylocta-1,7-diene(dl)	262	C20H22	1010215-92-8	25
5	4-(3,5-Dimethyl-1H-pyrazol-1-yl)...	187	C11H13N3	052708-32-4	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070623\
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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...	2.140	46.3	ng	1579000	1	6.846	682660	20.0
2-Pentanone, 4-...	5.093	2.7	ng	91296	1	6.846	682660	20.0
Benzophenone	10.598	4.9	ng	189944	3	9.881	773172	20.0
n-Hexadecanoic ...	11.910	14.0	ng	437293	4	11.375	622816	20.0
Phenol, 2-[(4-h...	12.204	2.7	ng	83055	4	11.375	622816	20.0
Phenol, 2,2'-me...	12.457	3.2	ng	99187	4	11.375	622816	20.0
Tetradecanoic acid	12.704	7.0	ng	217591	4	11.375	622816	20.0
(1R,4aR,4bS,7S,...	13.175	2.8	ng	92504	5	14.039	667620	20.0