LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

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-BF071317.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	4.792	472	477	484	rBV	183114	262790	12.08%	1.319%
2	4.881	484	492	497	rVV2	14985	28882	1.33%	0.145%
3	5.228	547	551	565	rBV	2187925	2151430	98.93%	10.797%
4	6.269	723	728	740	rBV	2108954	2174687	100.00%	10.914%
5	6.386	744	748	751	rBV	2404215	2096832	96.42%	10.523%
6	6.610	783	786	790	rBV	695951	584816	26.89%	2.935%
7	6.769	809	813	816	rBV	1857134	1597734	73.47%	8.018%
8	7.175	877	882	885	rBV	1399124	1276435	58.70%	6.406%
9	7.892	1000	1004	1007	rBV	979921	765839	35.22%	3.843%
10	8.969	1182	1187	1190	rBV	2321653	1990749	91.54%	9.991%
11	9.304	1241	1244	1247	rBV	41982	32869	1.51%	0.165%
12	9.363	1250	1254	1257	rBV	199511	172511	7.93%	0.866%
13	9.639	1295	1301	1304	rBV	785642	687083	31.59%	3.448%
14	10.021	1362	1366	1370	rBV	43786	32204	1.48%	0.162%
15	10.086	1374	1377	1380	rVV	43175	33165	1.53%	0.166%
16	10.310	1408	1415	1417	rBV	15881	24886	1.14%	0.125%
17	10.421	1430	1434	1438	rBV	971753	849342	39.06%	4.262%
18	10.557	1454	1457	1464	rBV	47948	57105	2.63%	0.287%
19	11.110	1548	1551	1554	rBV	533305	487481	22.42%	2.446%
20	11.621	1635	1638	1642	rBV	49612	55554	2.55%	0.279%
21	11.663	1642	1645	1652	rVB2	94275	99691	4.58%	0.500%
22	12.315	1752	1756	1759	rVB	114763	101975	4.69%	0.512%
23	12.421	1771	1774	1776	rBV3	30405	22942	1.05%	0.115%
24	12.539	1790	1794	1797	rBV	51992	57960	2.67%	0.291%
25	12.580	1797	1801	1805	rVV2	38336	48088	2.21%	0.241%
26	12.698	1816	1821	1824	rBV	1389433	1328466	61.09%	6.667%
27	12.786	1834	1836	1840	rVB5	32962	28756	1.32%	0.144%
28	12.880	1849	1852	1856	rVB	90413	75100	3.45%	0.377%
29	12.915	1856	1858	1860	rBV3	29956	28523	1.31%	0.143%
30	13.068	1881	1884	1887	rBV	109461	89917	4.13%	0.451%
31	13.174	1896	1902	1905	rBV6	45579	50662	2.33%	0.254%
32	13.280	1915	1920	1924	rVB5	74271	94801	4.36%	0.476%
33	13.386	1934	1938	1941	rVB2	69948	63444	2.92%	0.318%
34	13.568	1966	1969	1972	rBV2	55042	60489	2.78%	0.304%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.604	1972	1975	1980	rVB2	142899	173708	7.99%	0.872%
36	13.739	1993	1998	2001	rBV	602699	628576	28.90%	3.154%
37	13.774	2001	2004	2009	rVB2	117621	123488	5.68%	0.620%
38	13.927	2027	2030	2032	rBV	27865	26726	1.23%	0.134%
39	13.992	2038	2041	2046	rBV5	53236	59870	2.75%	0.300%
40	14.033	2046	2048	2053	rBV5	29247	36790	1.69%	0.185%
41	14.080	2053	2056	2061	rVV6	28316	38938	1.79%	0.195%
42	14.233	2078	2082	2087	rBV	93942	115075	5.29%	0.578%
43	14.586	2140	2142	2145	rVB	41258	37605	1.73%	0.189%
44	14.733	2164	2167	2169	rBV2	32609	32891	1.51%	0.165%
45	14.821	2179	2182	2190	rBV	138488	198320	9.12%	0.995%
46	15.109	2227	2231	2236	rBV	422284	484679	22.29%	2.432%
47	15.539	2300	2304	2309	rBV	320708	456460	20.99%	2.291%

Sum of corrected areas: 19926334

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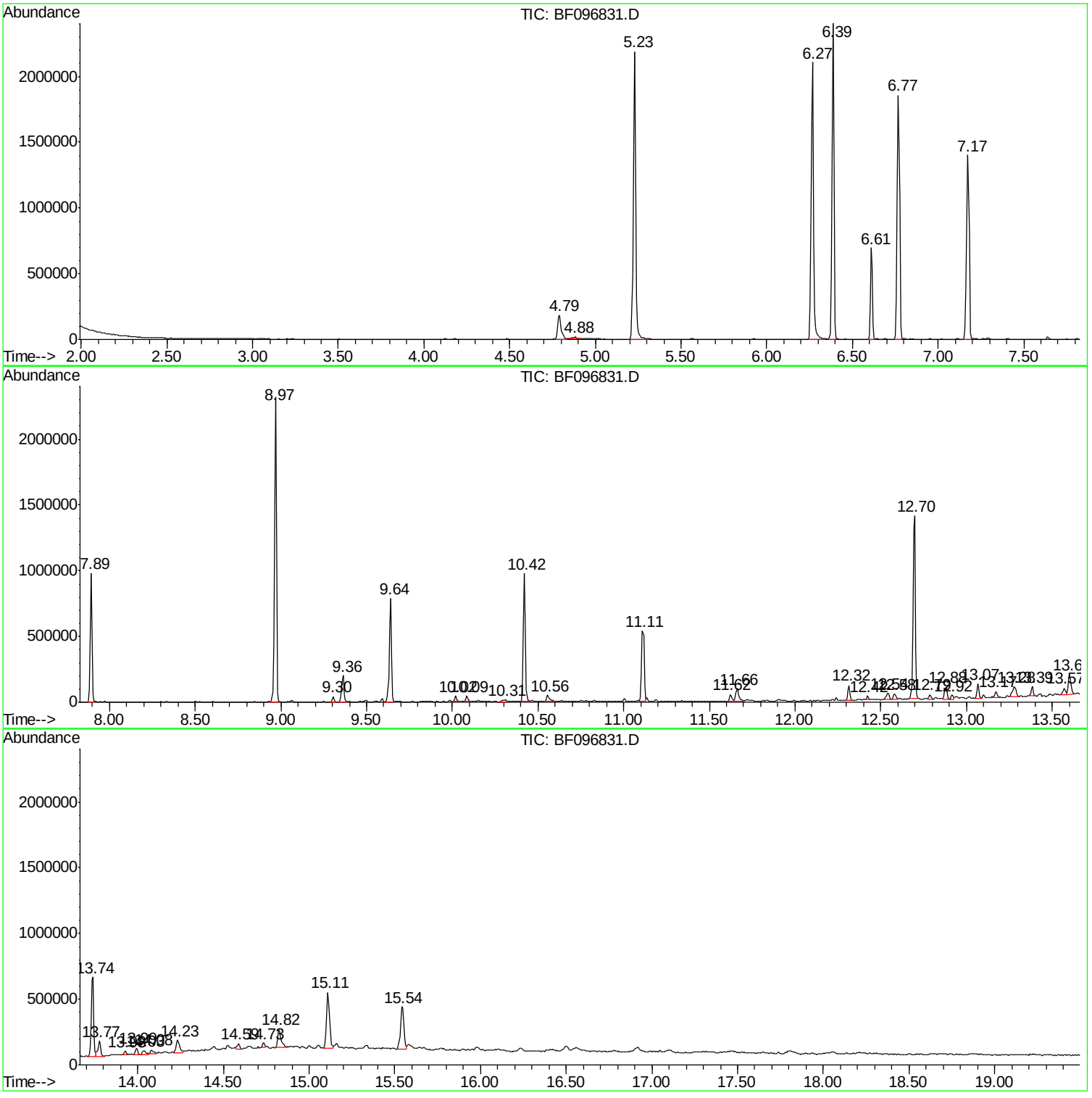
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

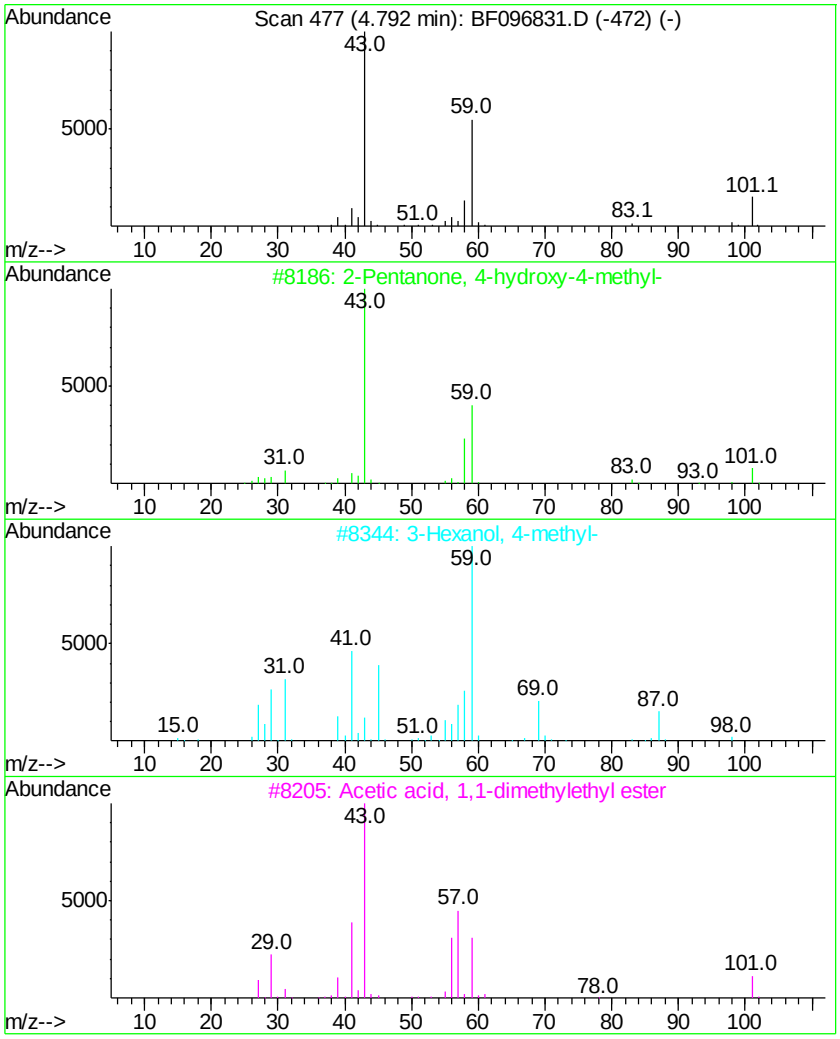
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

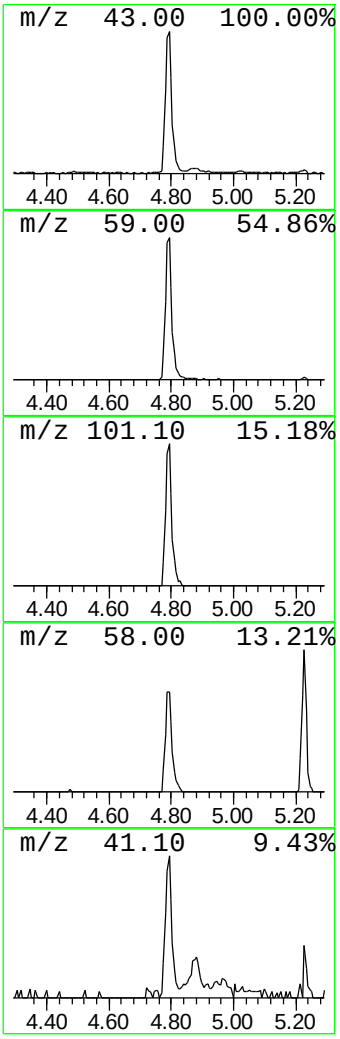
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	8.99 ng	262790	1,4-Dichlorobenzene-d4	6.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

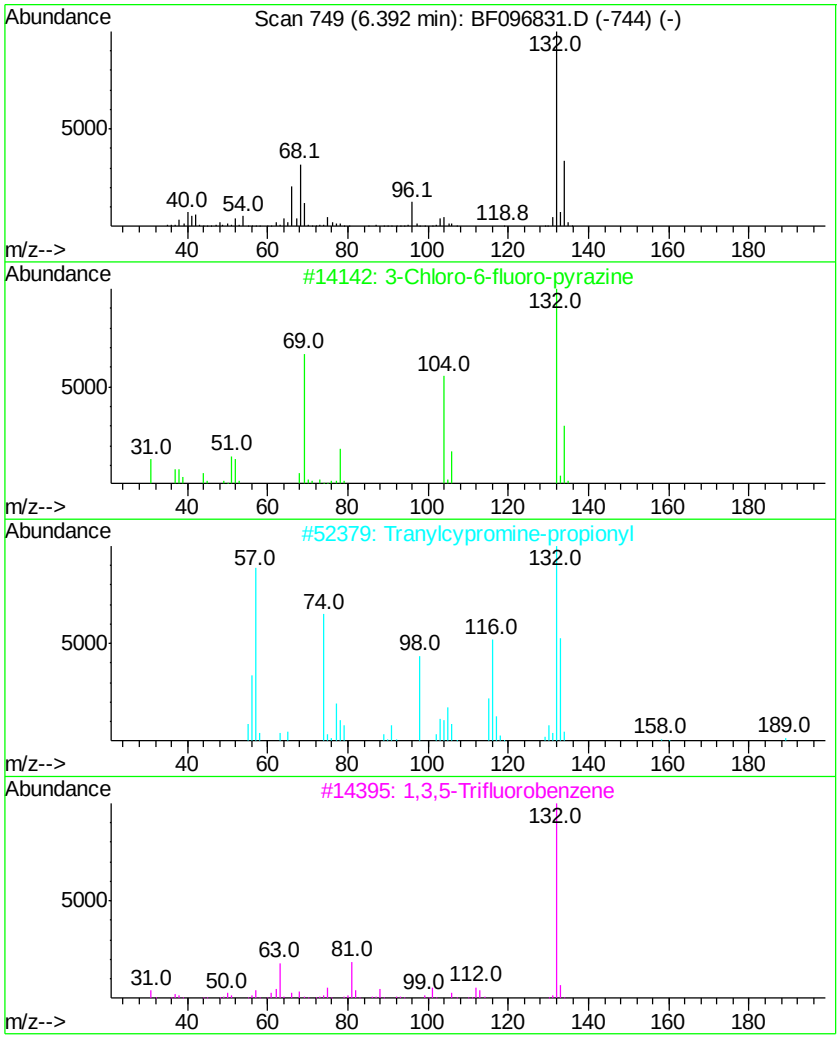
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

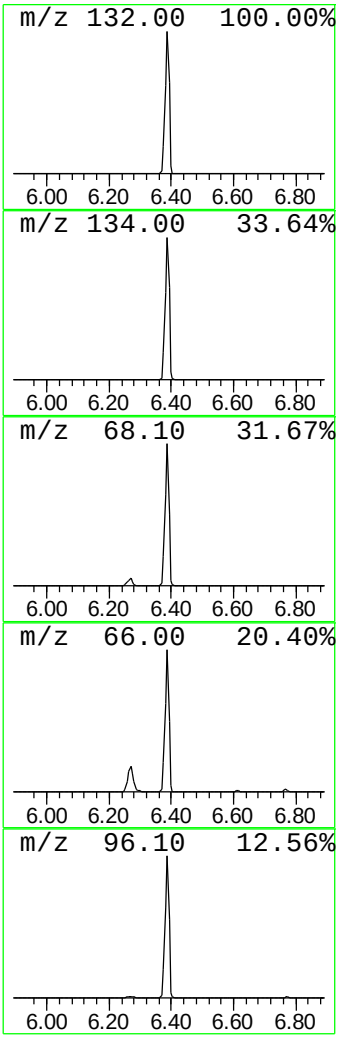
****

Peak Number 2 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	71.71 ng	2096830	1,4-Dichlorobenzene-d4	6.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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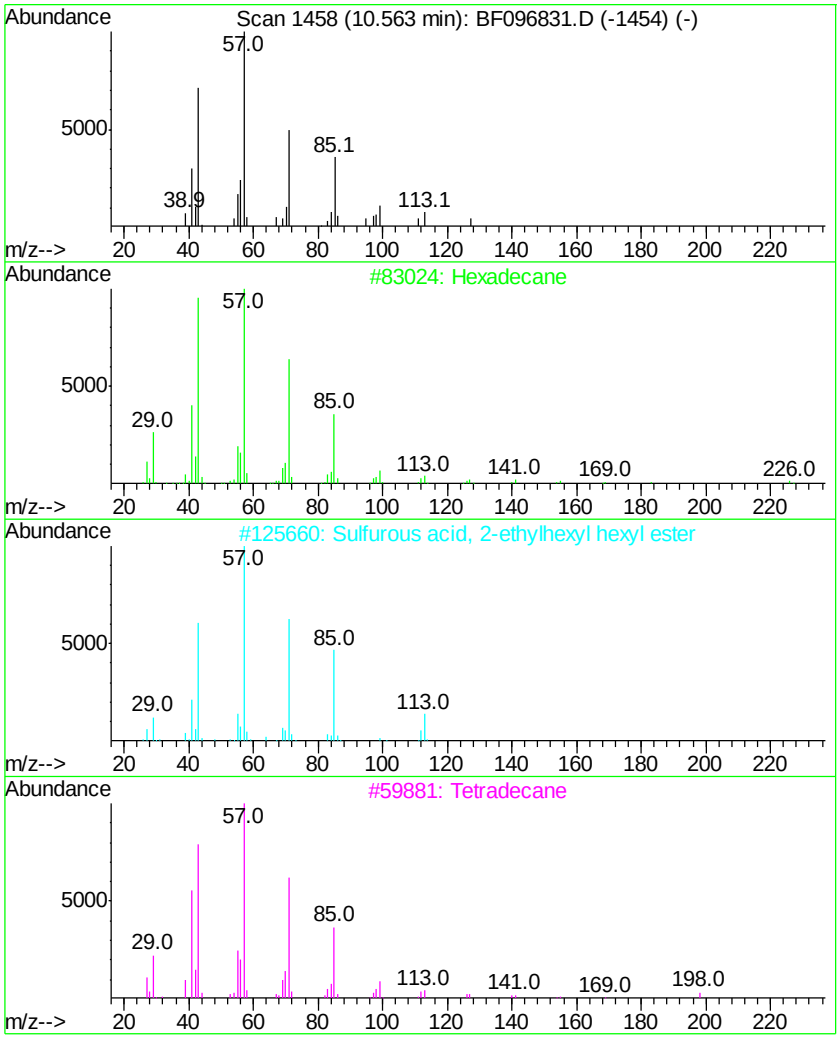
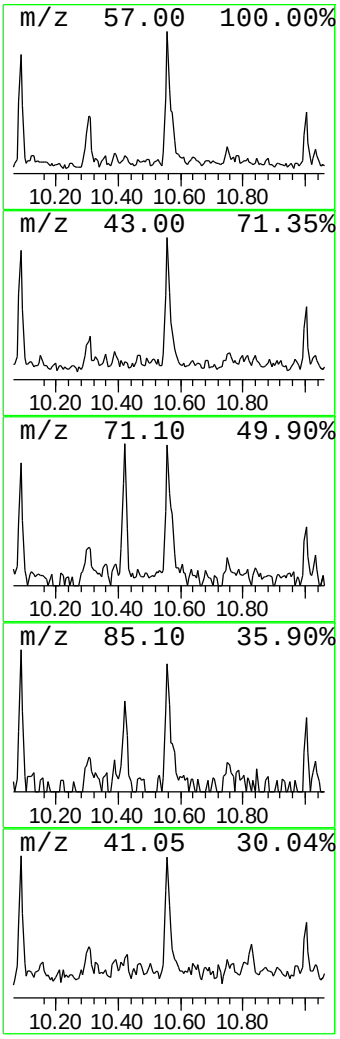
Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.34 ng	57105	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	86
3	Tetradecane	198	C14H30	000629-59-4	72
4	Tridecane	184	C13H28	000629-50-5	72
5	Pentadecane	212	C15H32	000629-62-9	72





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Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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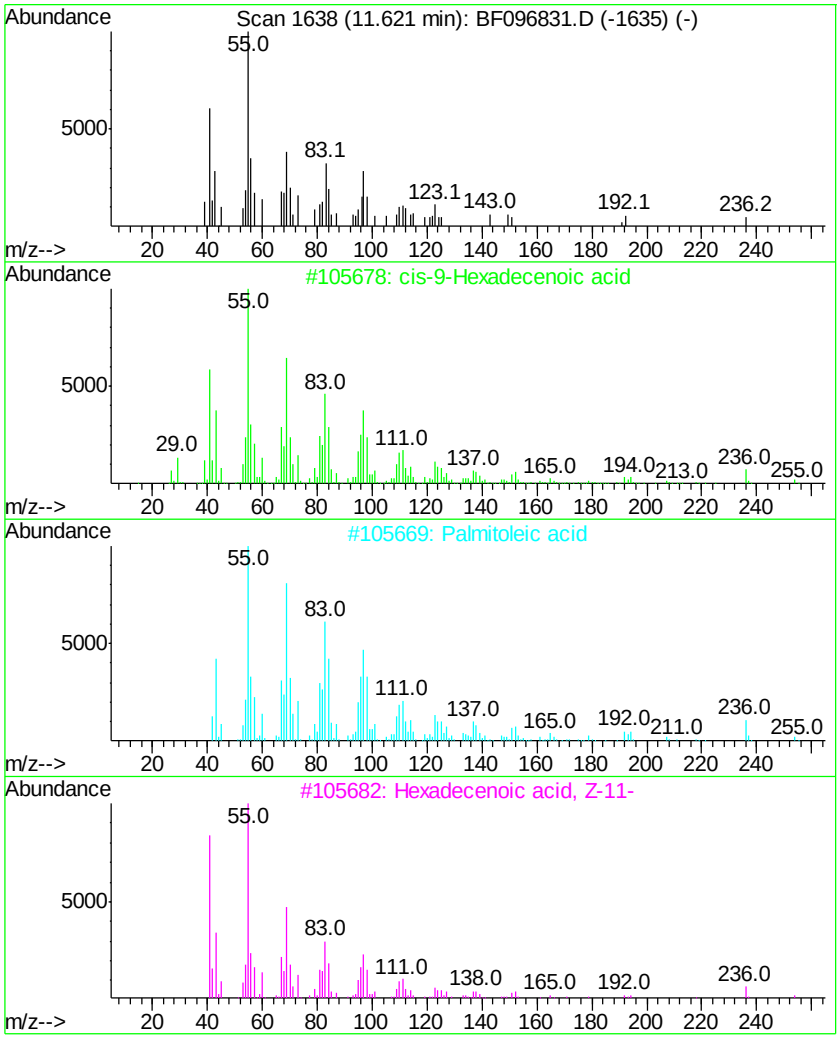
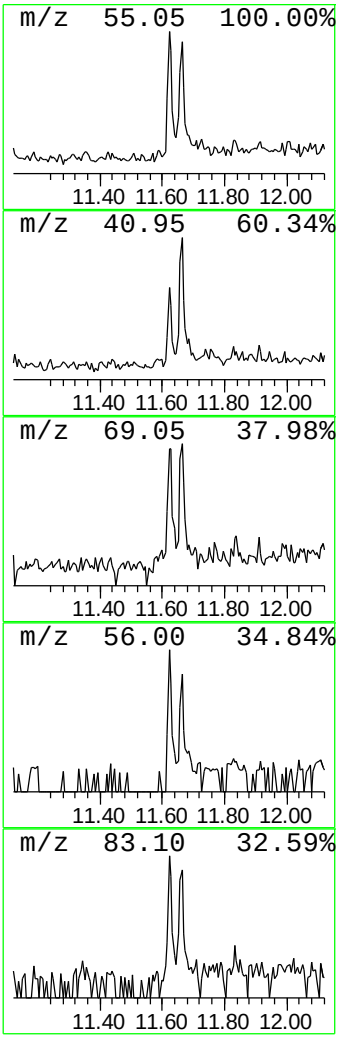
Peak Number 5 cis-9-Hexadecenoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	2.28 ng	55554	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	87
2	Palmitoleic acid	254	C16H30O2	000373-49-9	83
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	58
4	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	49
5	E-9-Tetradecenoic acid	226	C14H26O2	1000131-35-8	49





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

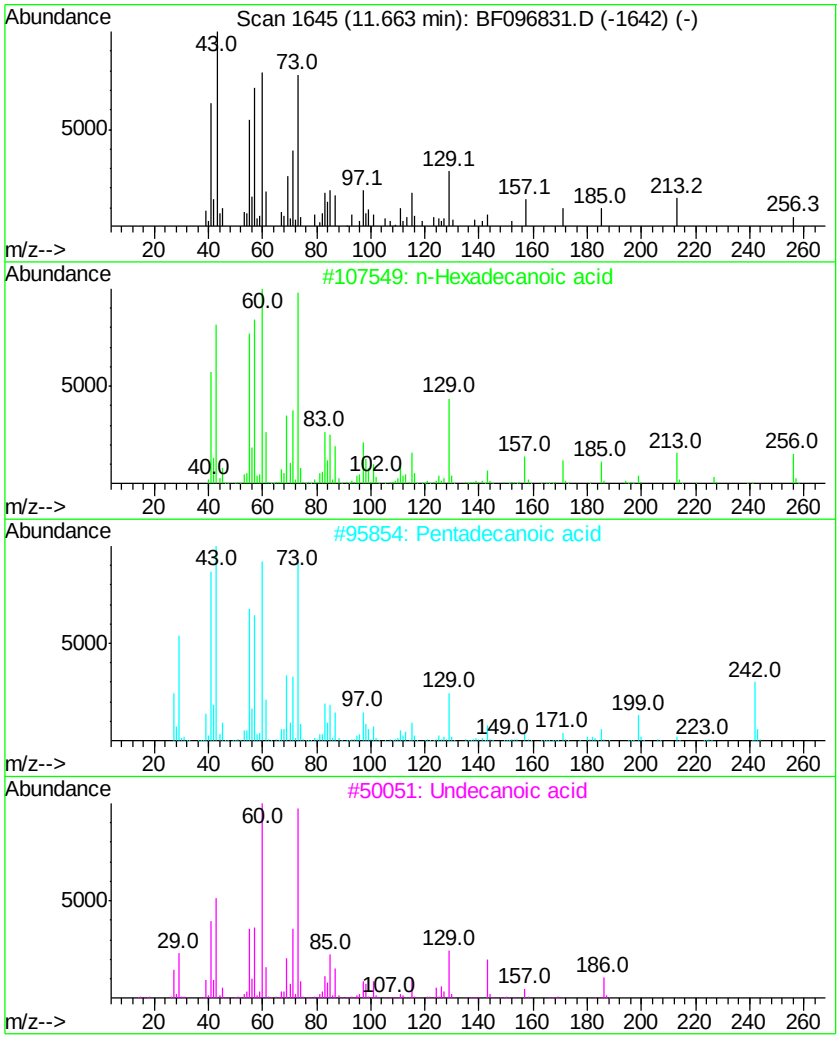
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

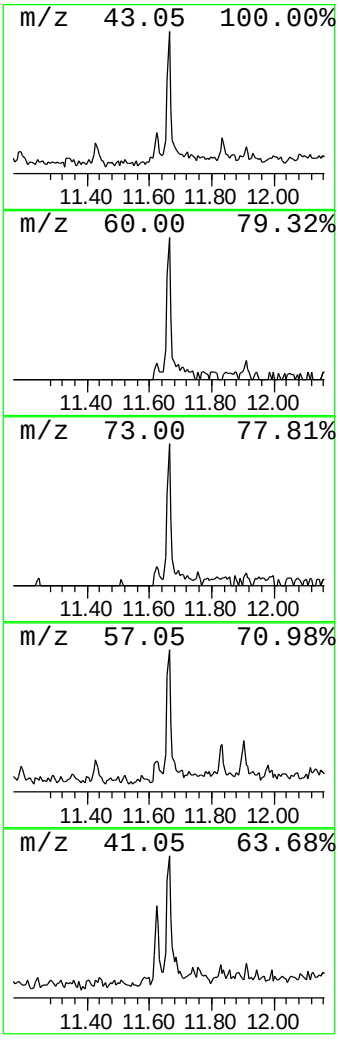
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	4.09 ng	99691	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

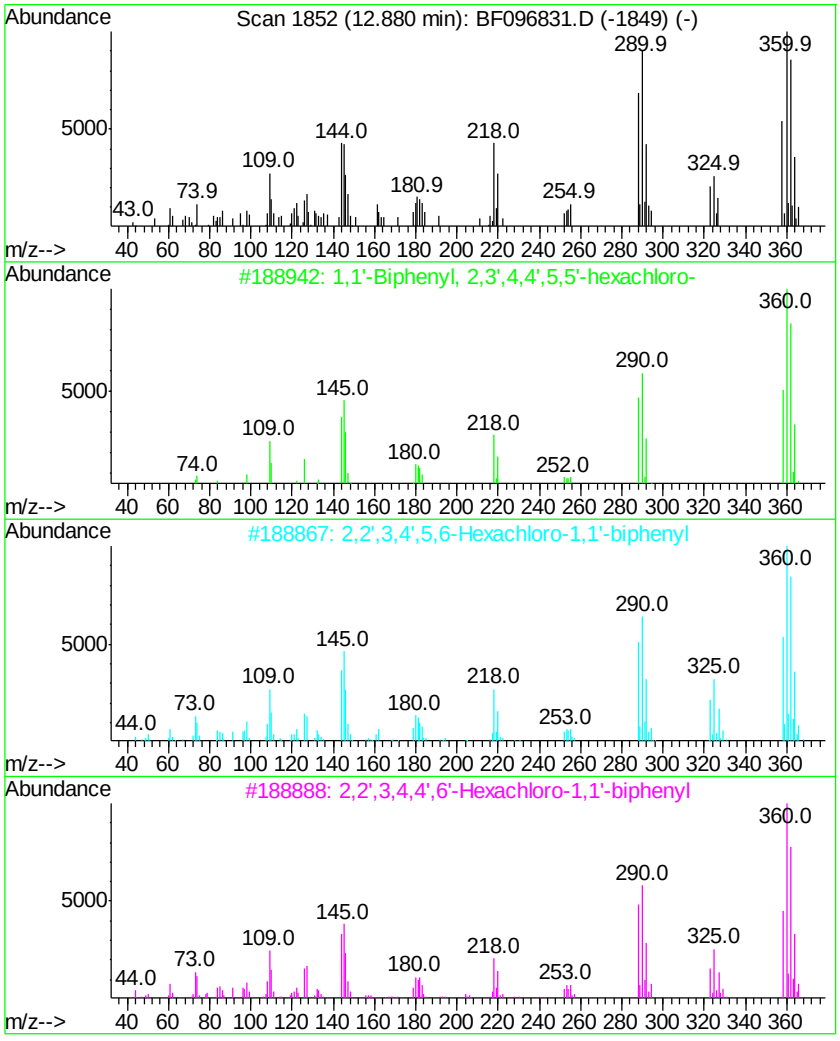
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

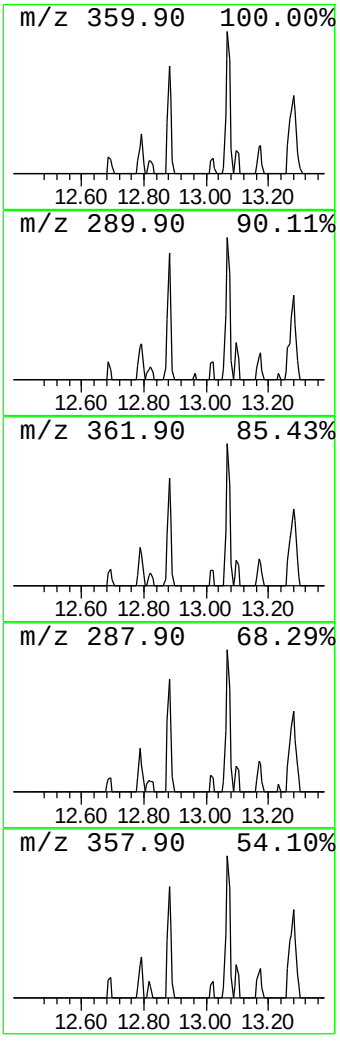
****

Peak Number 8 1,1'-Biphenyl, 2,3',4,4',5,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.88	2.39 ng	75100	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,3',4,4',5,5'-he...	358	C12H4Cl6	052663-72-6	99
2	2,2',3,4',5,6-Hexachloro-1,1'-bi...	358	C12H4Cl6	068194-13-8	99
3	2,2',3,4,4',6'-Hexachloro-1,1'-b...	358	C12H4Cl6	059291-64-4	99
4	1,1'-Biphenyl, 2,2',4,4',5',6-He...	358	C12H4Cl6	060145-22-4	99
5	1,1'-Biphenyl, 2,2',3,4,4',6-Hex...	358	C12H4Cl6	056030-56-9	99





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

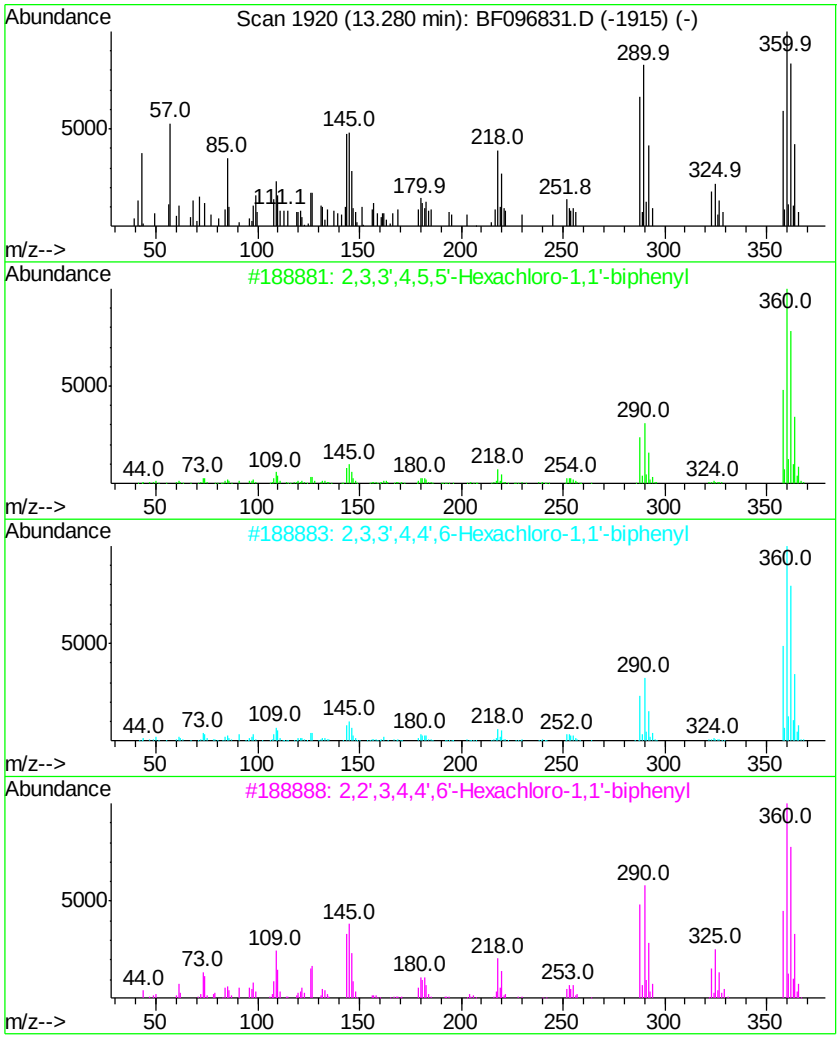
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

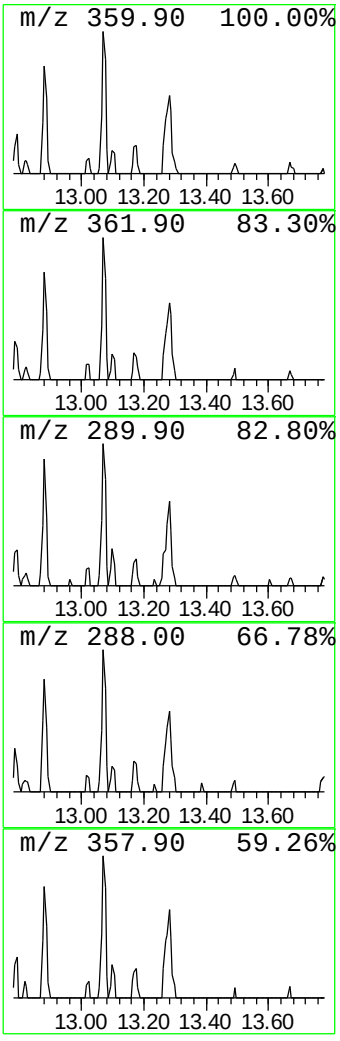
****

Peak Number 10 2,3,3',4,5,5'-Hexachloro-1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	3.02 ng	94801	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,3',4,5,5'-Hexachloro-1,1'-bi...	358	C12H4Cl6	039635-35-3	99
2	2,3,3',4,4',6-Hexachloro-1,1'-bi...	358	C12H4Cl6	074472-42-7	99
3	2,2',3,4,4',6'-Hexachloro-1,1'-b...	358	C12H4Cl6	059291-64-4	99
4	1,1'-Biphenyl, 2,2',3,4,5,5'-hex...	358	C12H4Cl6	052712-04-6	99
5	1,1'-Biphenyl, 2,3,3',4,5,6-hexa...	358	C12H4Cl6	041411-62-5	99





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

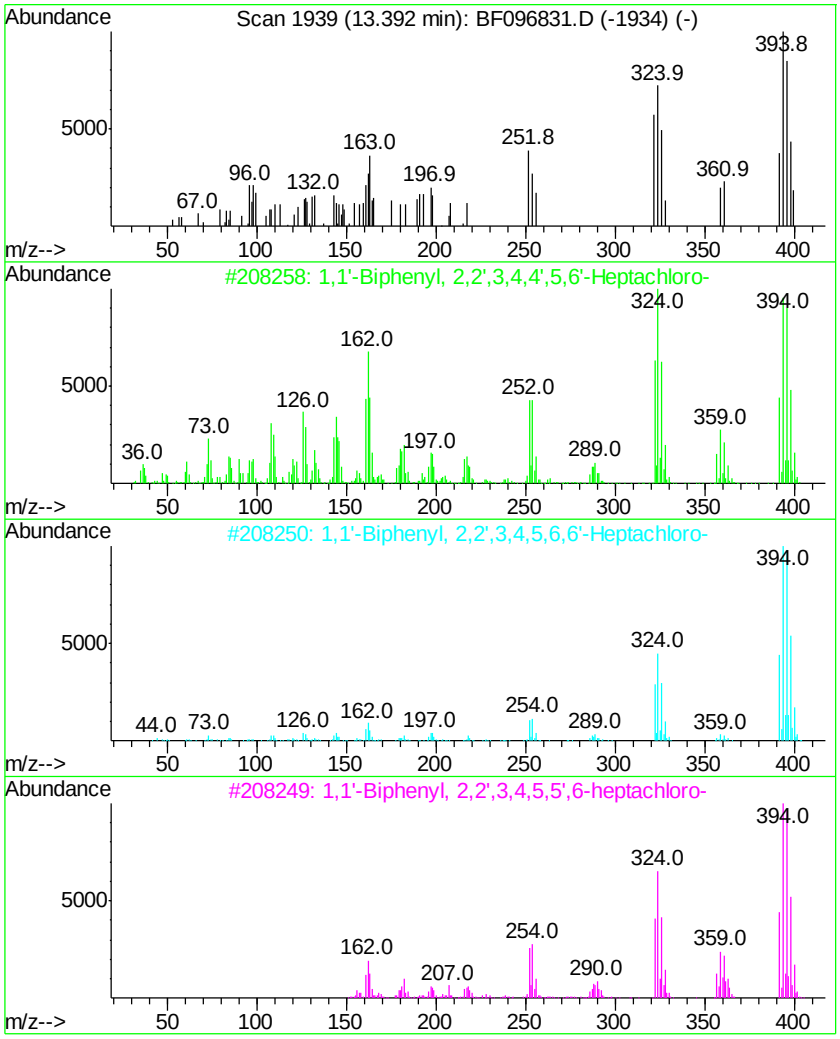
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

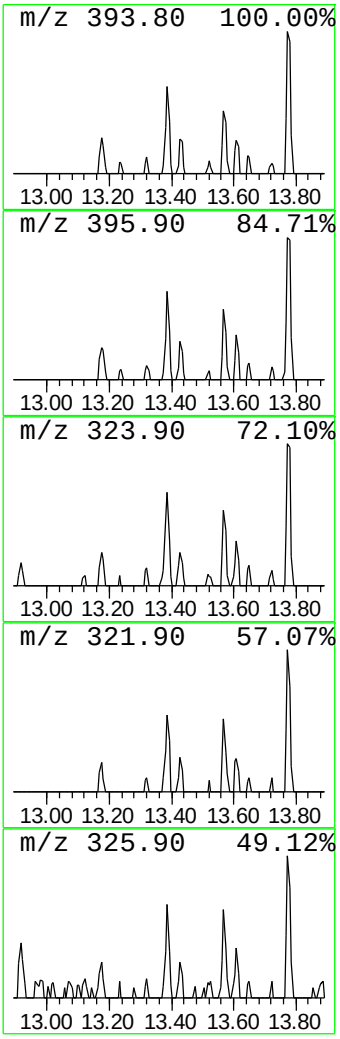
****

Peak Number 11 1,1'-Biphenyl, 2,2',3,4,4',... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	2.02 ng	63444	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 2,2',3,4,4',5,6'-...	392	C12H3Cl7	060145-23-5	99
2	1,1'-Biphenyl, 2,2',3,4,5,6,6'-H...	392	C12H3Cl7	074472-49-4	99
3	1,1'-Biphenyl, 2,2',3,4,5,5',6-h...	392	C12H3Cl7	052712-05-7	99
4	1,1'-Biphenyl, 2,3,3',4,4',5,6-H...	392	C12H3Cl7	041411-64-7	99
5	1,1'-Biphenyl, 2,2',3,3',4,4',5-...	392	C12H3Cl7	035065-30-6	99





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Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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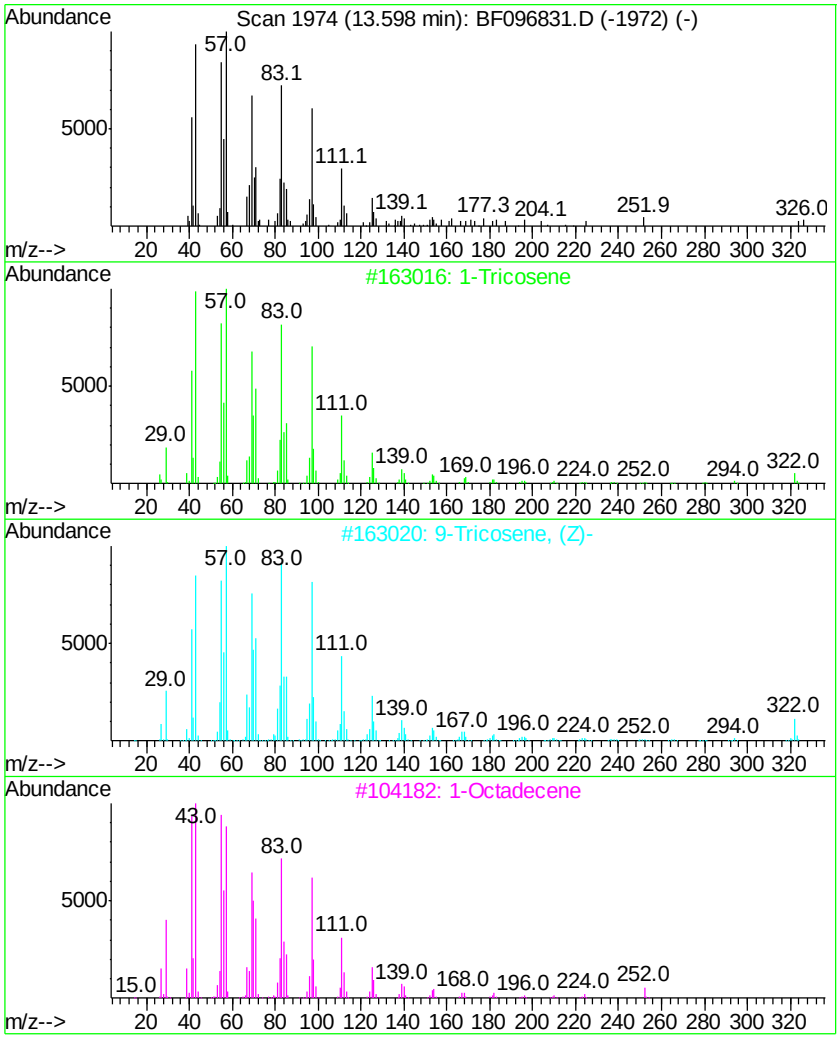
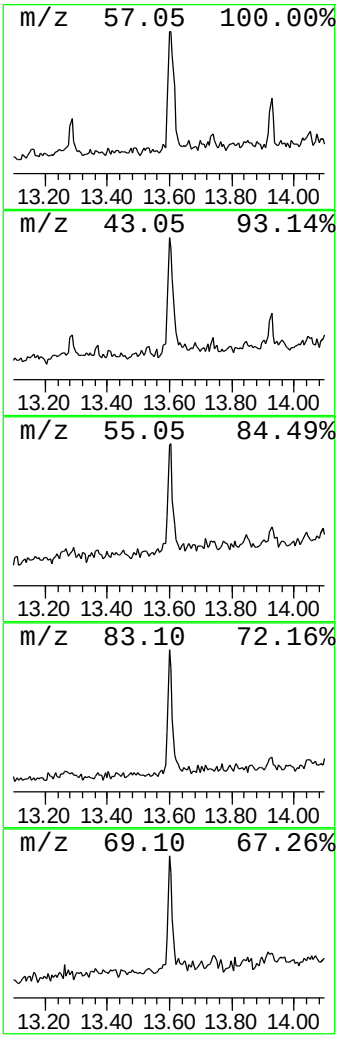
Peak Number 12 1-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	5.53 ng	173708	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	99
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	96
3	1-Octadecene	252	C18H36	000112-88-9	94
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5	Cyclooctacosane	392	C28H56	000297-24-5	91





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Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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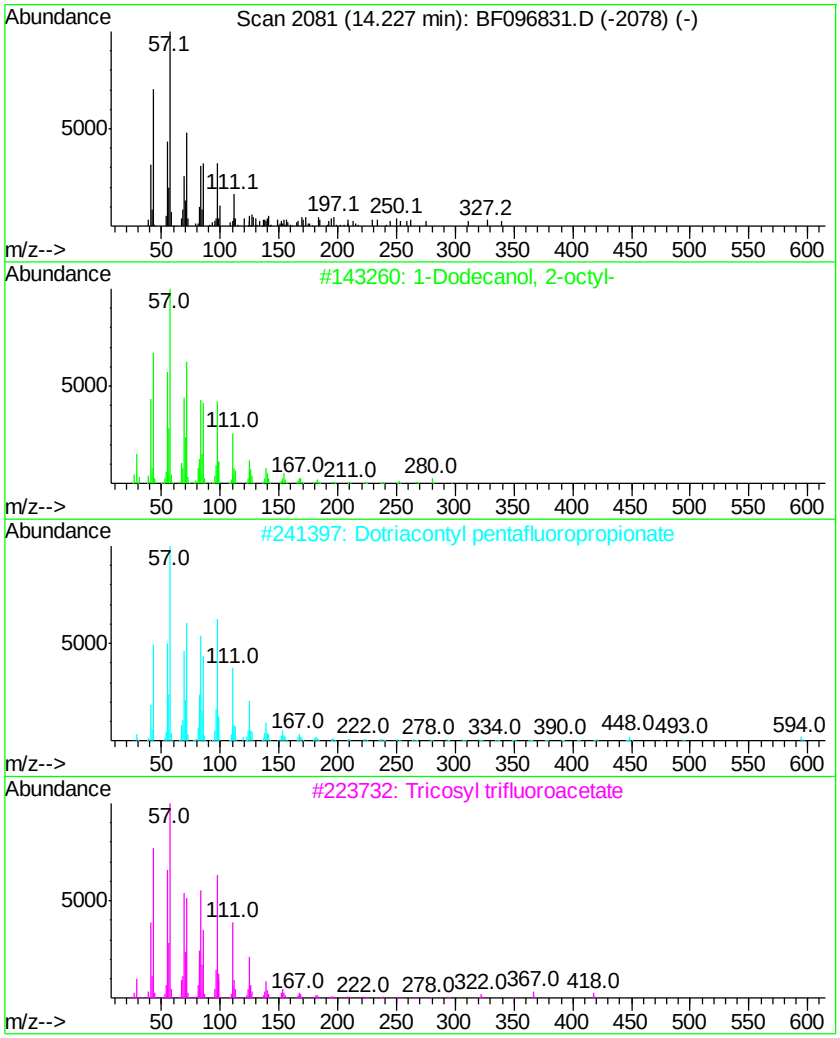
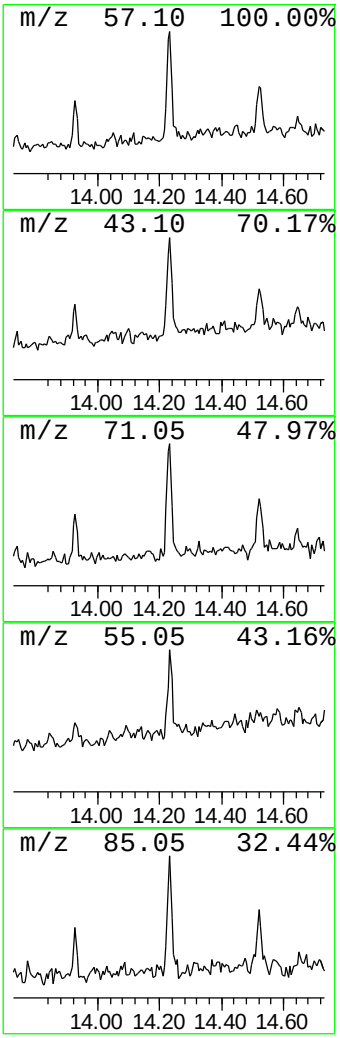
Peak Number 13 1-Dodecanol, 2-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	3.66 ng	115075	Chrysene-d12	13.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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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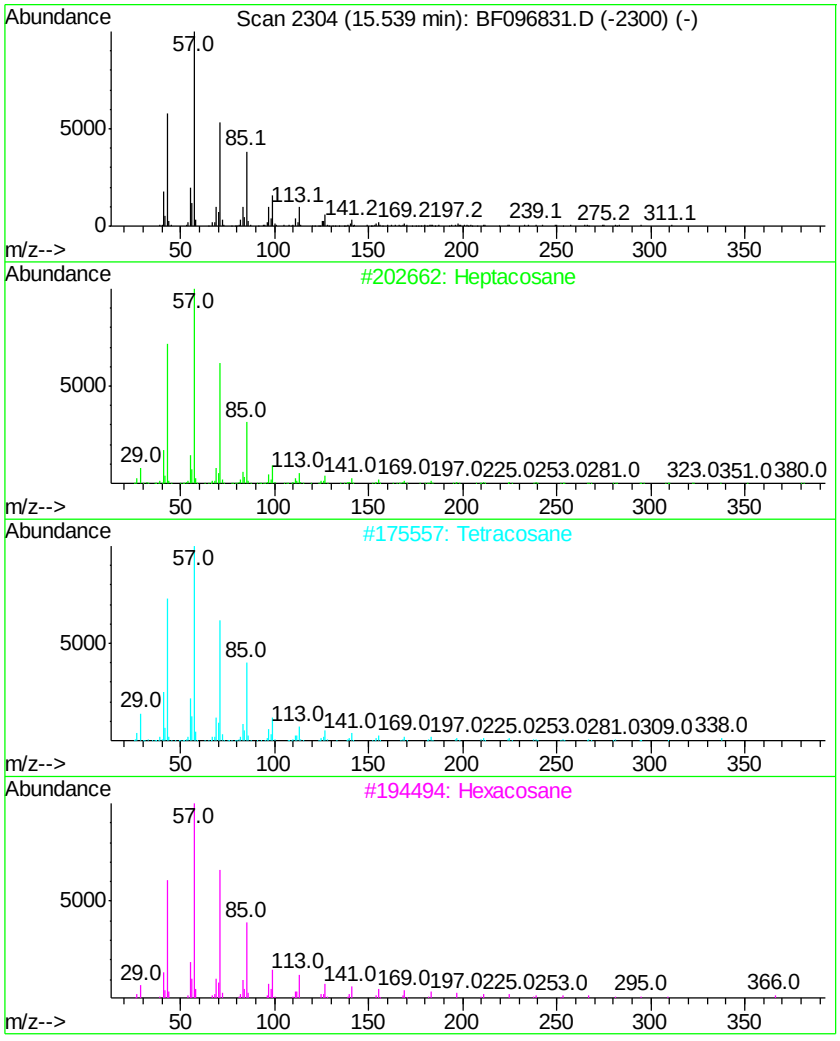
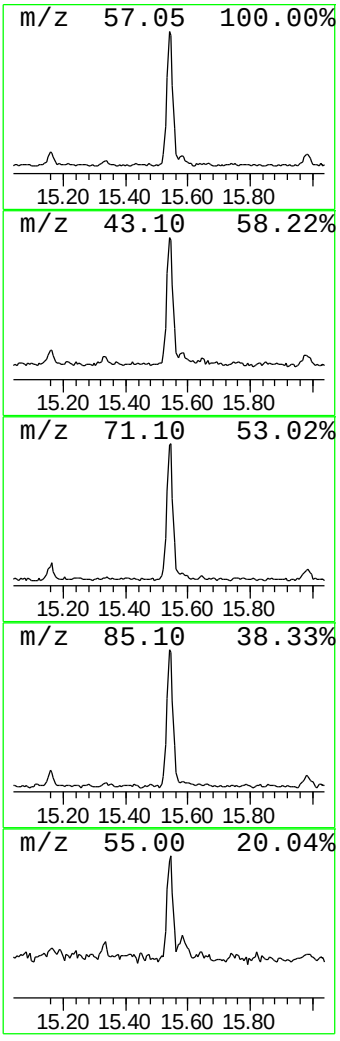
Peak Number 15 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	18.84 ng	456460	Perylene-d12	15.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octadecane	254	C18H38	000593-45-3	86
5	Hexadecane	226	C16H34	000544-76-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
Data File : BF096831.D
Acq On : 17 Jul 2017 20:42
Operator : SJ/JU
Sample : I4203-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-SB01A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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
2-Pentanone, 4-hy...	4.79	9.0	ng	262790	1	6.61	584816	20.0
unknown6.39	6.39	71.7	ng	2096830	1	6.61	584816	20.0
Hexadecane	10.56	2.3	ng	57105	4	11.11	487481	20.0
cis-9-Hexadecenoi...	11.62	2.3	ng	55554	4	11.11	487481	20.0
n-Hexadecanoic acid	11.66	4.1	ng	99691	4	11.11	487481	20.0
1,1'-Biphenyl, 2,...	12.88	2.4	ng	75100	5	13.74	628576	20.0
2,3,3',4,5,5'-Hex...	13.28	3.0	ng	94801	5	13.74	628576	20.0
1,1'-Biphenyl, 2,...	13.39	2.0	ng	63444	5	13.74	628576	20.0
1-Tricosene	13.60	5.5	ng	173708	5	13.74	628576	20.0
1-Dodecanol, 2-oc...	14.23	3.7	ng	115075	5	13.74	628576	20.0
Heptacosane	15.54	18.8	ng	456460	6	15.11	484679	20.0