LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021021\
Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-020921

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123178.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	14	rVB	205105	265612	8.93%	0.866%
2	3.598	250	257	262	rVB	23823	40434	1.36%	0.132%
3	3.734	274	280	288	rVB	19931	34338	1.15%	0.112%
4	5.492	575	579	582	rBV	2015106	1718387	57.76%	5.602%
5	6.498	746	750	758	rBV	1787172	1804845	60.66%	5.884%
6	6.716	783	787	790	rBV2	28745	34411	1.16%	0.112%
7	6.881	812	815	822	rVB	1275595	1022232	34.36%	3.332%
8	7.439	906	910	913	rBV	1385655	1115667	37.50%	3.637%
9	7.481	915	917	921	rVB	67686	51242	1.72%	0.167%
10	8.163	1027	1033	1036	rBV	1418681	1386500	46.60%	4.520%
11	8.228	1040	1044	1047	rVB3	31358	35956	1.21%	0.117%
12	8.463	1078	1084	1090	rBV6	22605	35252	1.18%	0.115%
13	8.757	1131	1134	1138	rBV	90297	69573	2.34%	0.227%
14	8.880	1152	1155	1158	rVB	42354	34406	1.16%	0.112%
15	8.980	1168	1172	1176	rBV2	40265	43112	1.45%	0.141%
16	9.239	1212	1216	1220	rBV	2463205	2183646	73.39%	7.119%
17	9.322	1226	1230	1233	rBV	95655	91252	3.07%	0.297%
18	9.357	1233	1236	1241	rVV	135710	140953	4.74%	0.460%
19	9.580	1271	1274	1276	rBV	38751	34245	1.15%	0.112%
20	9.633	1281	1283	1287	rVV	139204	125287	4.21%	0.408%
21	9.786	1305	1309	1314	rBV	44270	44066	1.48%	0.144%
22	9.857	1314	1321	1324	rBV	78643	76230	2.56%	0.249%
23	9.927	1329	1333	1336	rVV	1779989	1558675	52.39%	5.081%
24	9.957	1336	1338	1342	rVB	69574	53139	1.79%	0.173%
25	10.127	1363	1367	1372	rVB2	34142	35607	1.20%	0.116%
26	10.357	1403	1406	1408	rVB	76260	61803	2.08%	0.201%
27	10.474	1422	1426	1431	rVB	73332	77275	2.60%	0.252%
28	10.580	1438	1444	1447	rVB4	25735	39730	1.34%	0.130%
29	10.710	1461	1466	1474	rBV	997542	899696	30.24%	2.933%
30	10.827	1483	1486	1491	rBV2	69629	91674	3.08%	0.299%
31	11.280	1560	1563	1565	rBV	61786	48385	1.63%	0.158%
32	11.310	1565	1568	1573	rVB	59377	63474	2.13%	0.207%
33	11.416	1582	1586	1588	rBV	1773865	1471778	49.47%	4.798%
34	11.439	1588	1590	1593	rVV	451690	333488	11.21%	1.087%
35	11.492	1596	1599	1602	rVB	101635	97733	3.28%	0.319%
36	11.710	1633	1636	1638	rBV	66754	55615	1.87%	0.181%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021021\
Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-020921

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.810	1649	1653	1656	rBV	1137039	892140	29.99%	2.908%
38	11.916	1668	1671	1672	rBV	87433	72811	2.45%	0.237%
39	11.945	1672	1676	1683	rVV	913340	1129210	37.95%	3.681%
40	12.033	1687	1691	1693	rVV2	144761	195485	6.57%	0.637%
41	12.080	1697	1699	1703	rVV	60620	54584	1.83%	0.178%
42	12.116	1703	1705	1710	rVB	53762	51494	1.73%	0.168%
43	12.216	1719	1722	1724	rBV	43529	34793	1.17%	0.113%
44	12.468	1762	1765	1767	rBV	70200	75697	2.54%	0.247%
45	12.498	1767	1770	1772	rVV	3317936	2975239	100.00%	9.699%
46	12.521	1772	1774	1784	rVB	2461854	2131889	71.65%	6.950%
47	12.604	1785	1788	1790	rBV	408106	318062	10.69%	1.037%
48	12.633	1790	1793	1796	rVV	377428	310386	10.43%	1.012%
49	12.739	1806	1811	1818	rBV	1306704	1761703	59.21%	5.743%
50	12.863	1826	1832	1834	rBV	370735	364412	12.25%	1.188%
51	13.004	1852	1856	1860	rBV	2237212	1874365	63.00%	6.110%
52	13.168	1881	1884	1885	rBV2	39349	38788	1.30%	0.126%
53	13.192	1885	1888	1892	rVB	87666	83961	2.82%	0.274%
54	13.239	1893	1896	1897	rBV	46171	42952	1.44%	0.140%
55	13.257	1897	1899	1901	rVB	80005	64694	2.17%	0.211%
56	13.292	1903	1905	1908	rBV2	60247	56738	1.91%	0.185%
57	13.386	1919	1921	1924	rBV	34550	34200	1.15%	0.111%
58	13.421	1924	1927	1929	rBV	41150	35768	1.20%	0.117%
59	14.062	2032	2036	2039	rBV	1306398	1308958	44.00%	4.267%
60	14.086	2039	2040	2049	rVB	147936	130369	4.38%	0.425%
61	15.115	2211	2215	2218	rBV2	133570	234652	7.89%	0.765%
62	15.551	2284	2289	2293	rBV	899322	1125652	37.83%	3.670%

Sum of corrected areas: 30674720

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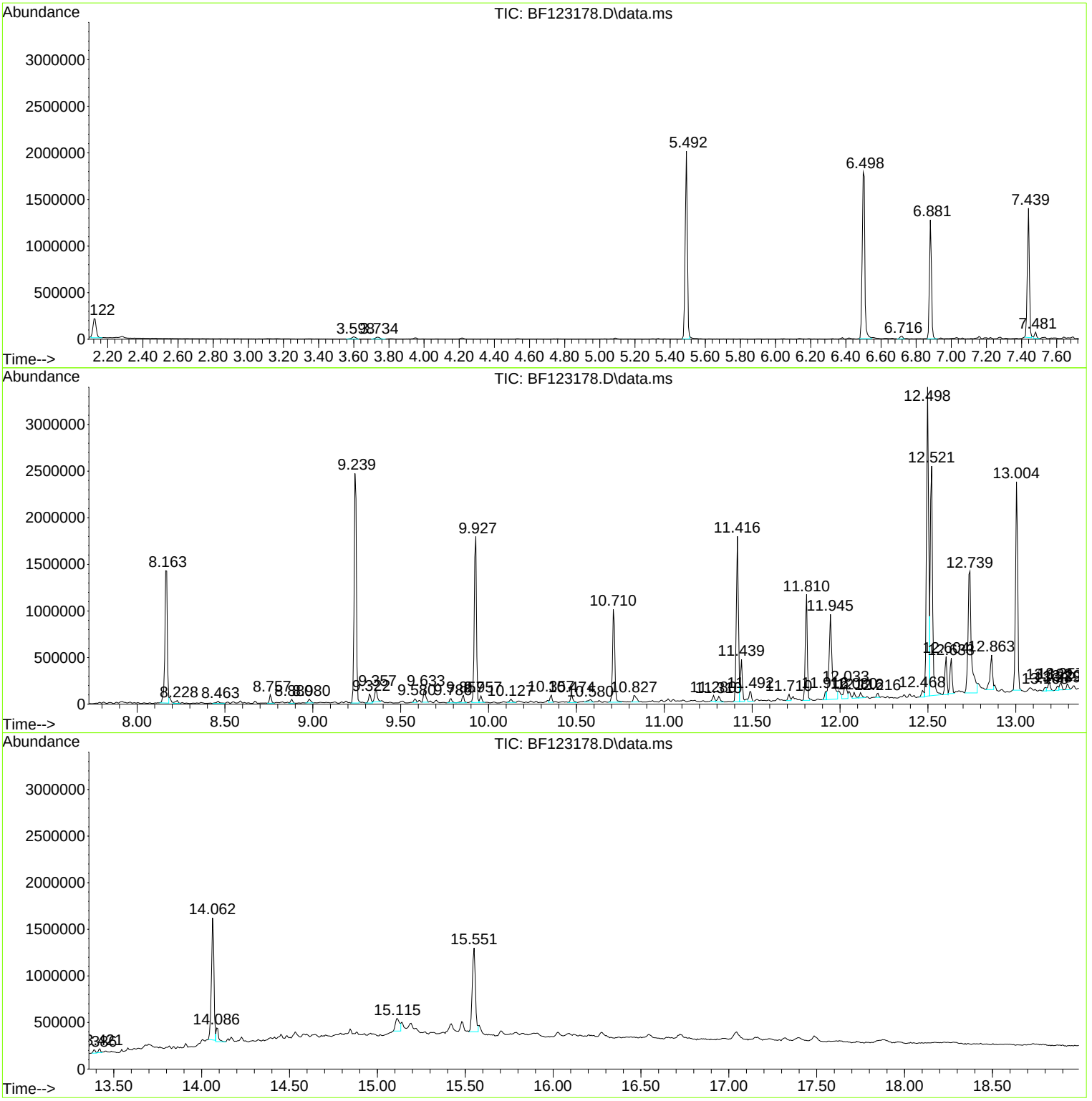
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-020921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021021\
Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-020921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

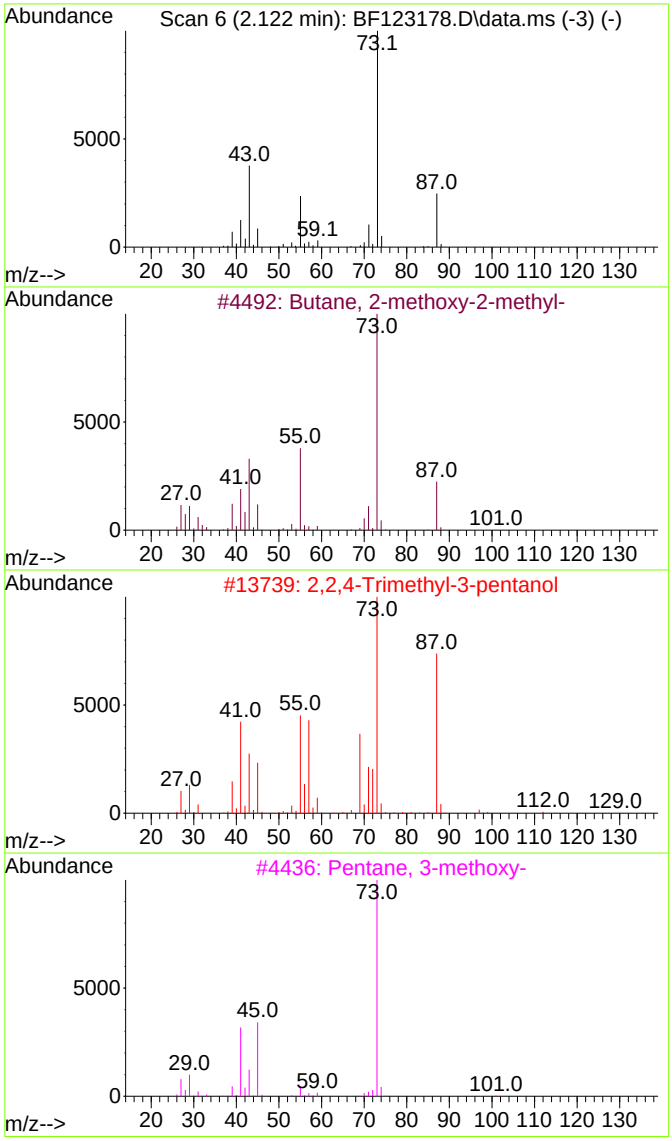
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

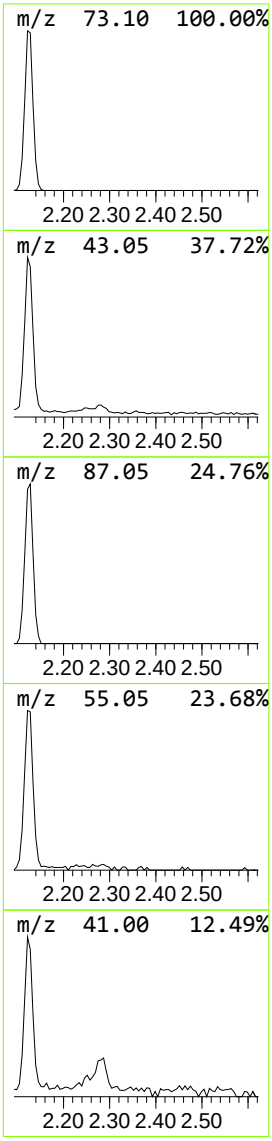
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	5.20 ng	265612	1,4-Dichlorobenzene-d4	6.881

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021021\
Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-020921

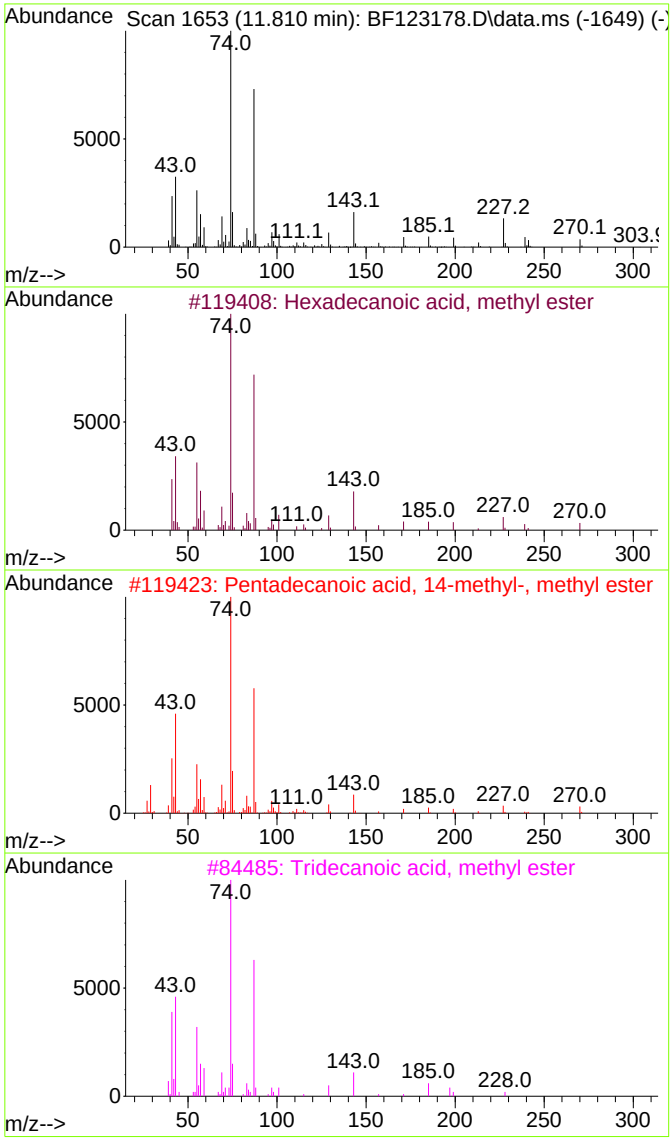
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

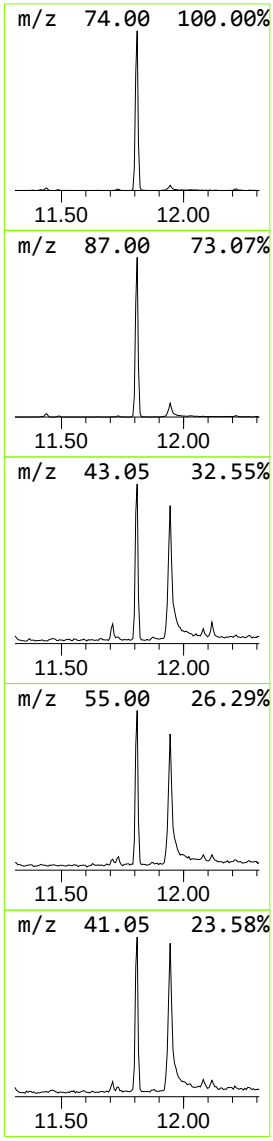
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	12.12 ng	892140	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	83
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021021\
Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EO-03-020921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

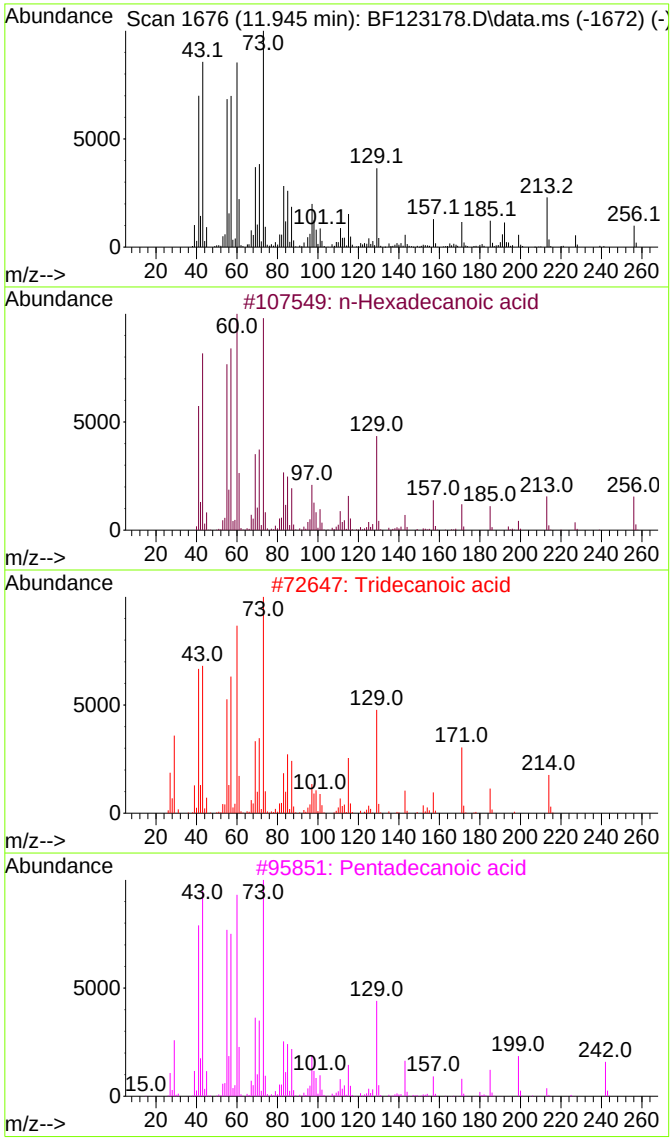
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

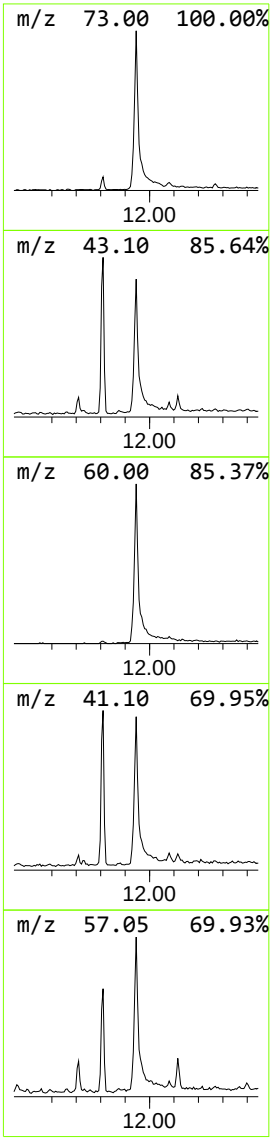
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	15.34 ng	1129210	Phenanthrene-d10	11.416

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021021\
Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-020921

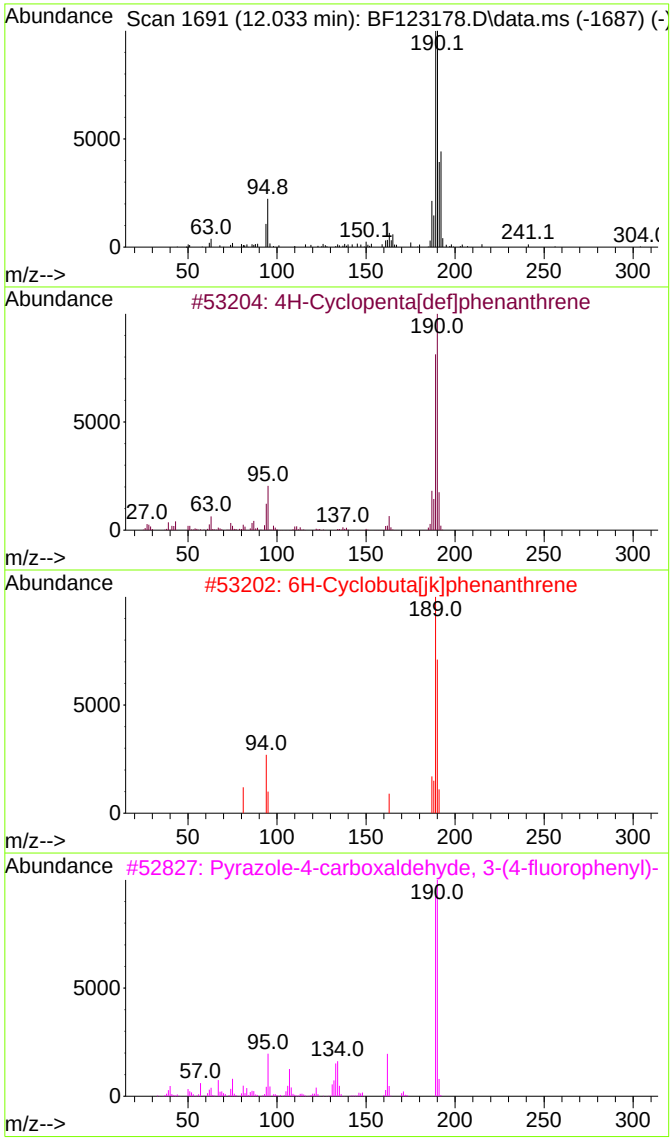
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

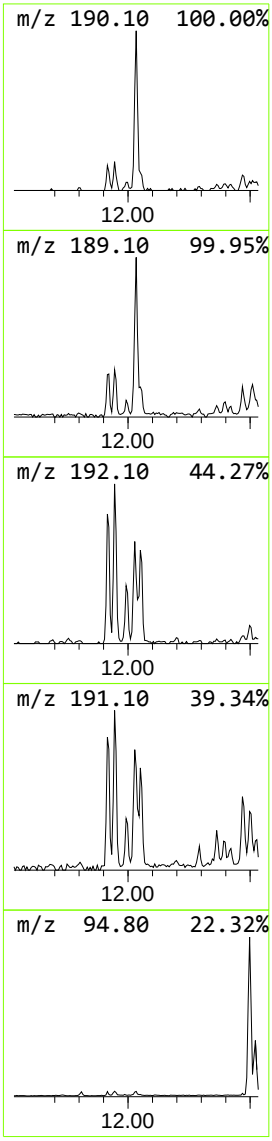
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.66 ng	195485	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	46
5	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	40





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Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-020921

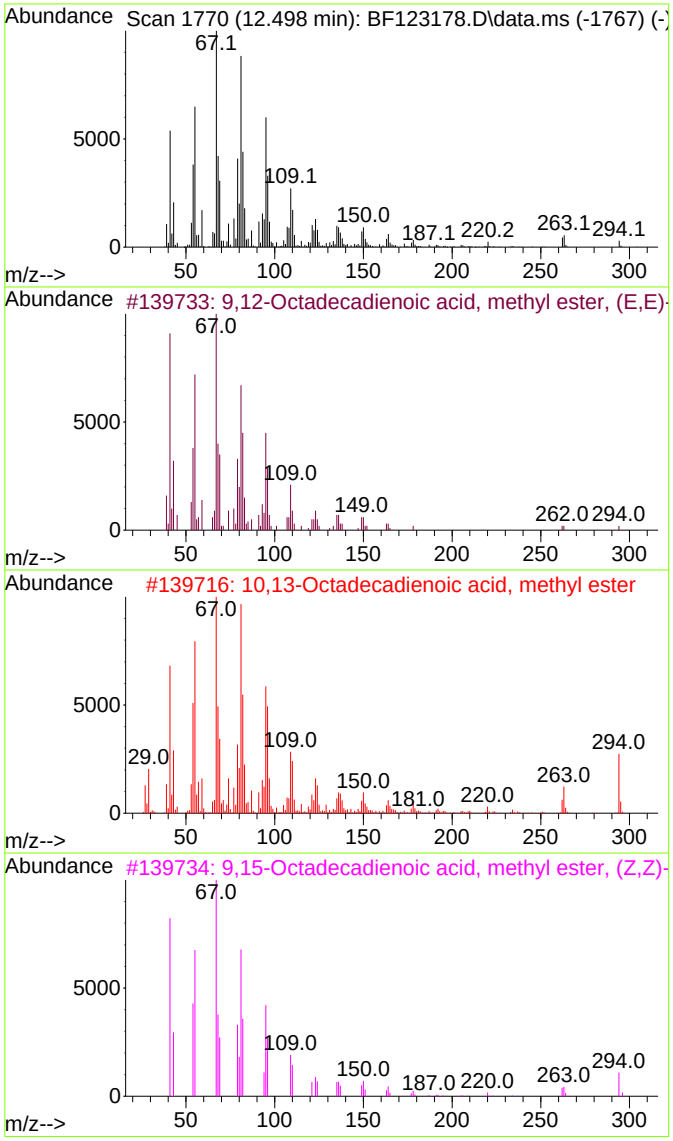
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

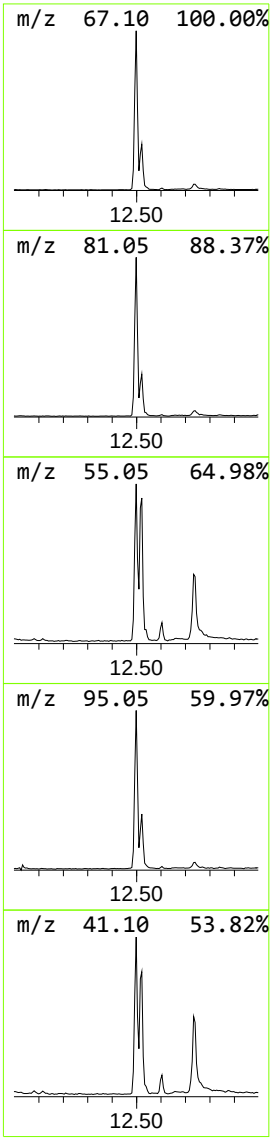
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	40.43 ng	2975240	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





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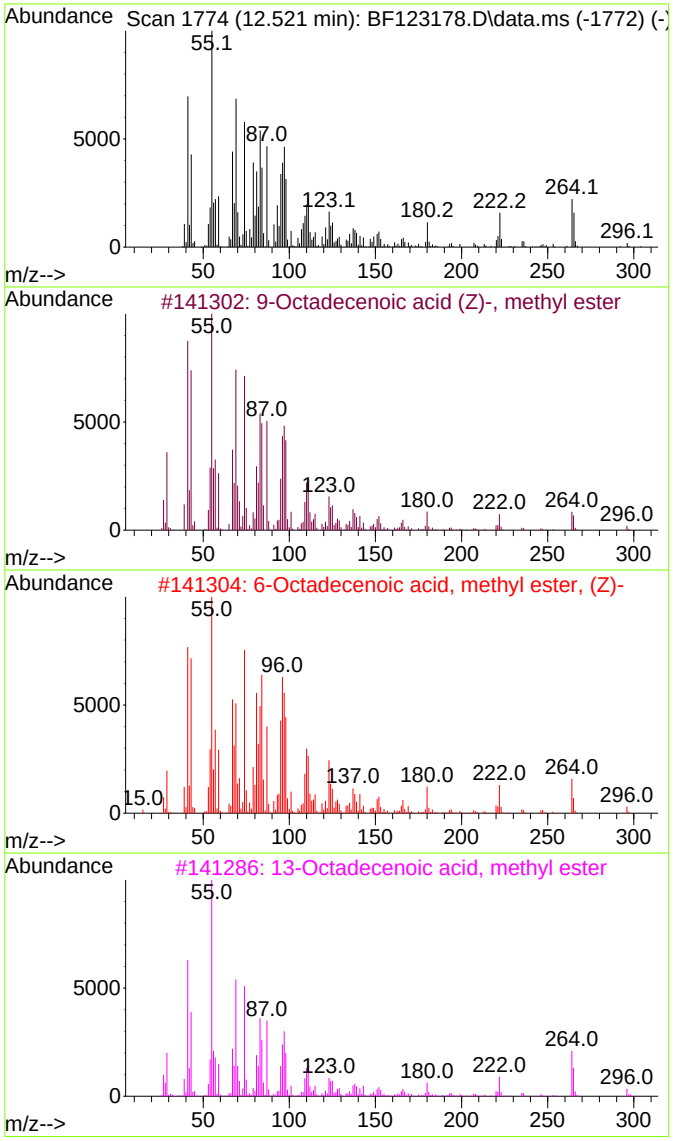
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

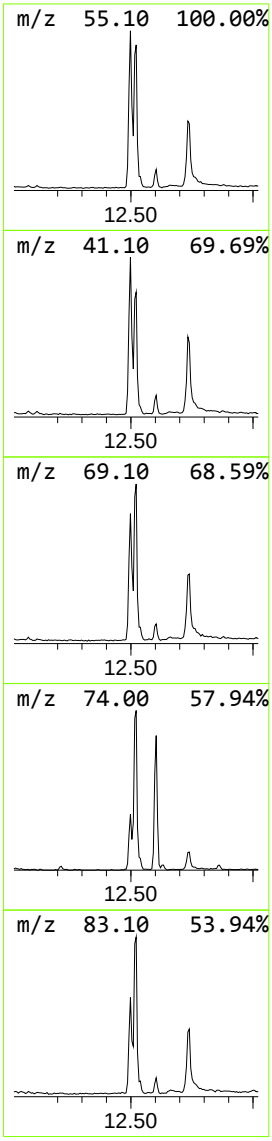
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.521	28.97 ng	2131890	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
4	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99





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Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-020921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

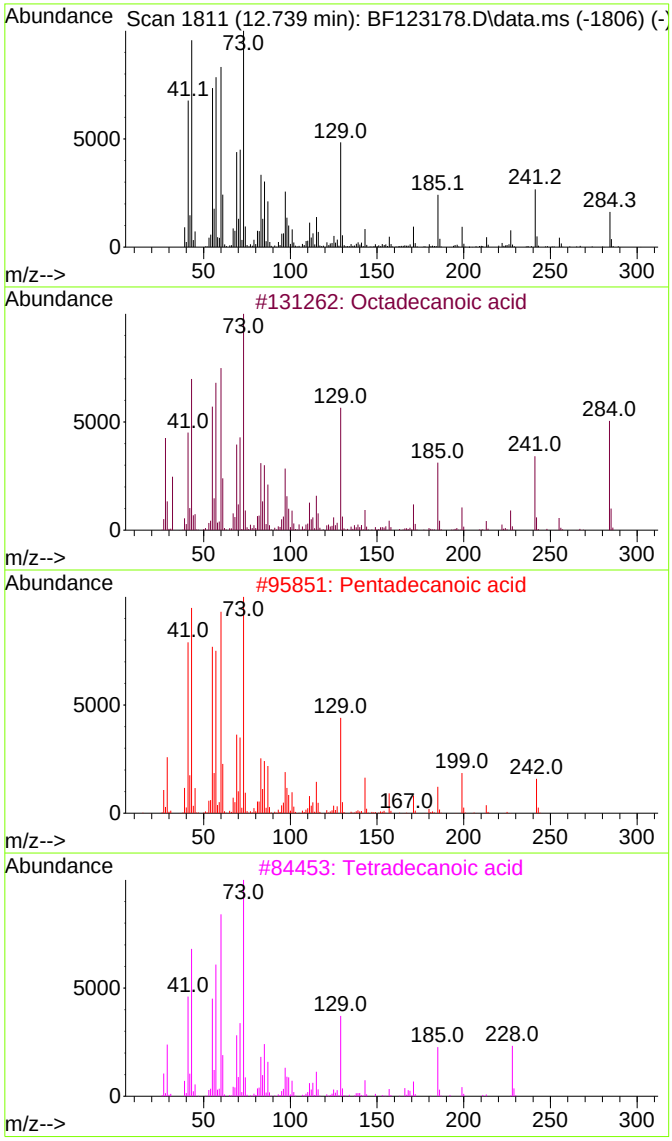
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

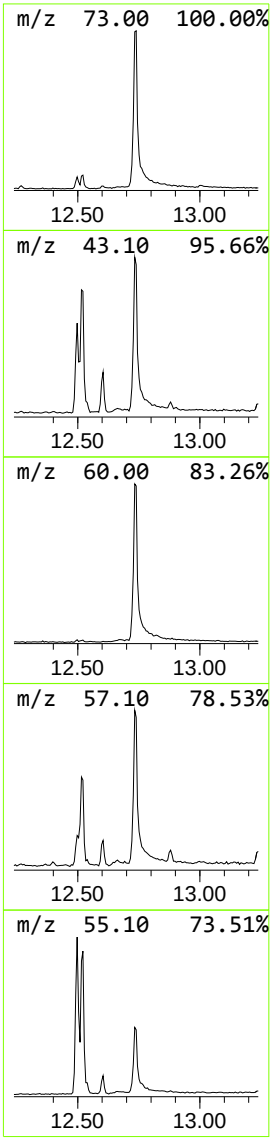
****

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	23.94 ng	1761700	Phenanthrene-d10	11.416

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	Tridecanoic acid	214	C13H26O2	000638-53-9	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021021\
Data File : BF123178.D
Acq On : 10 Feb 2021 19:28
Operator : JU/CG
Sample : M1346-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EO-03-020921

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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
Butane, 2-metho...	2.122	5.2	ng	265612	1	6.881	1022230	20.0
Hexadecanoic ac...	11.810	12.1	ng	892140	4	11.416	1471780	20.0
n-Hexadecanoic ...	11.945	15.3	ng	1129210	4	11.416	1471780	20.0
4H-Cyclopenta[d...	12.033	2.7	ng	195485	4	11.416	1471780	20.0
9,12-Octadecadi...	12.498	40.4	ng	2975240	4	11.416	1471780	20.0
9-Octadecenoic ...	12.521	29.0	ng	2131890	4	11.416	1471780	20.0
Octadecanoic acid	12.739	23.9	ng	1761700	4	11.416	1471780	20.0