LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124990.D
Acq On : 8 Aug 2021 00:00
Operator : JU/CG
Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-080521

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124990.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.439	568	570	574	rBB	21522	16589	15.75%	2.647%
2	6.457	740	743	746	rBV	24740	17652	16.76%	2.817%
3	6.828	803	806	809	rBB	45853	36463	34.63%	5.818%
4	7.386	899	901	904	rBB	15628	11404	10.83%	1.820%
5	8.110	1021	1024	1028	rBB	55212	44291	42.06%	7.067%
6	9.186	1204	1207	1209	rBB	24092	18696	17.75%	2.983%
7	9.869	1319	1323	1325	rBB	52531	45614	43.32%	7.279%
8	10.651	1454	1456	1458	rBB	9690	5989	5.69%	0.956%
9	11.351	1572	1575	1578	rBV	55600	39668	37.67%	6.330%
10	11.739	1638	1641	1644	rBB	41626	29575	28.09%	4.719%
11	12.427	1754	1758	1760	rBV	117573	105301	100.00%	16.803%
12	12.451	1760	1762	1767	rVB	108248	88024	83.59%	14.046%
13	12.533	1773	1776	1778	rBB	14827	12392	11.77%	1.977%
14	12.563	1779	1781	1783	rBB	1940	1220	1.16%	0.195%
15	12.933	1841	1844	1847	rBB	19456	14698	13.96%	2.345%
16	13.680	1967	1971	1975	rBB	1504	1911	1.81%	0.305%
17	13.827	1994	1996	1997	rBV	1541	1157	1.10%	0.185%
18	13.986	2020	2023	2026	rBV	38319	35489	33.70%	5.663%
19	14.151	2047	2051	2053	rVB3	1179	1420	1.35%	0.227%
20	14.357	2083	2086	2090	rVB2	1061	1596	1.52%	0.255%
21	14.398	2090	2093	2097	rBV	2284	3067	2.91%	0.489%
22	14.445	2097	2101	2103	rVV2	2153	2088	1.98%	0.333%
23	14.480	2106	2107	2111	rVB	1239	1378	1.31%	0.220%
24	14.545	2114	2118	2119	rBV2	2172	2955	2.81%	0.472%
25	14.656	2134	2137	2139	rBV3	1241	1121	1.06%	0.179%
26	14.751	2149	2153	2156	rBV	1425	2041	1.94%	0.326%
27	14.898	2175	2178	2179	rVB2	2036	1511	1.43%	0.241%
28	14.951	2184	2187	2190	rVV5	1182	1621	1.54%	0.259%
29	15.021	2195	2199	2203	rBV3	2043	3846	3.65%	0.614%
30	15.080	2205	2209	2213	rVB2	1810	2762	2.62%	0.441%
31	15.168	2222	2224	2226	rVB2	1348	1121	1.06%	0.179%
32	15.192	2226	2228	2231	rBV3	1474	1529	1.45%	0.244%
33	15.233	2233	2235	2241	rVB3	987	1600	1.52%	0.255%
34	15.321	2247	2250	2252	rVB2	1077	1236	1.17%	0.197%
35	15.392	2259	2262	2264	rVB2	1370	1231	1.17%	0.196%
36	15.451	2268	2272	2277	rVB	24289	27980	26.57%	4.465%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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Acq On : 8 Aug 2021 00:00
Operator : JU/CG
Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-080521

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.486	2277	2278	2283	rBV3	1037	1217	1.16%	0.194%
38	15.580	2292	2294	2297	rVB2	1116	1197	1.14%	0.191%
39	15.645	2303	2305	2307	rVB3	1753	1127	1.07%	0.180%
40	15.845	2338	2339	2342	rBV2	1679	1484	1.41%	0.237%
41	15.886	2342	2346	2350	rVV3	2738	4169	3.96%	0.665%
42	16.127	2384	2387	2392	rBV4	1512	2522	2.40%	0.402%
43	16.292	2412	2415	2418	rBV3	1199	1322	1.26%	0.211%
44	16.386	2428	2431	2432	rBV2	2101	2084	1.98%	0.333%
45	16.498	2447	2450	2452	rBV2	905	1174	1.11%	0.187%
46	16.568	2457	2462	2466	rVB	2394	3967	3.77%	0.633%
47	16.650	2473	2476	2480	rBV	694	1483	1.41%	0.237%
48	16.680	2480	2481	2484	rVB2	1618	1244	1.18%	0.199%
49	16.768	2494	2496	2498	rVB	1208	1173	1.11%	0.187%
50	16.798	2498	2501	2503	rVB2	1481	1410	1.34%	0.225%
51	16.833	2503	2507	2508	rBV2	1108	1231	1.17%	0.196%
52	16.974	2525	2531	2533	rBV2	1326	2401	2.28%	0.383%
53	17.056	2541	2545	2546	rBV	1070	1507	1.43%	0.240%
54	17.286	2581	2584	2588	rBV	827	1411	1.34%	0.225%
55	17.639	2641	2644	2645	rBV2	1689	1779	1.69%	0.284%
56	17.656	2645	2647	2652	rVB2	1198	1653	1.57%	0.264%
57	17.980	2698	2702	2703	rBB2	1455	1265	1.20%	0.202%
58	18.121	2722	2726	2727	rBV	1106	1232	1.17%	0.197%
59	18.209	2738	2741	2744	rVB	849	1176	1.12%	0.188%
60	18.415	2773	2776	2778	rBV	1038	1222	1.16%	0.195%

Sum of corrected areas: 626686

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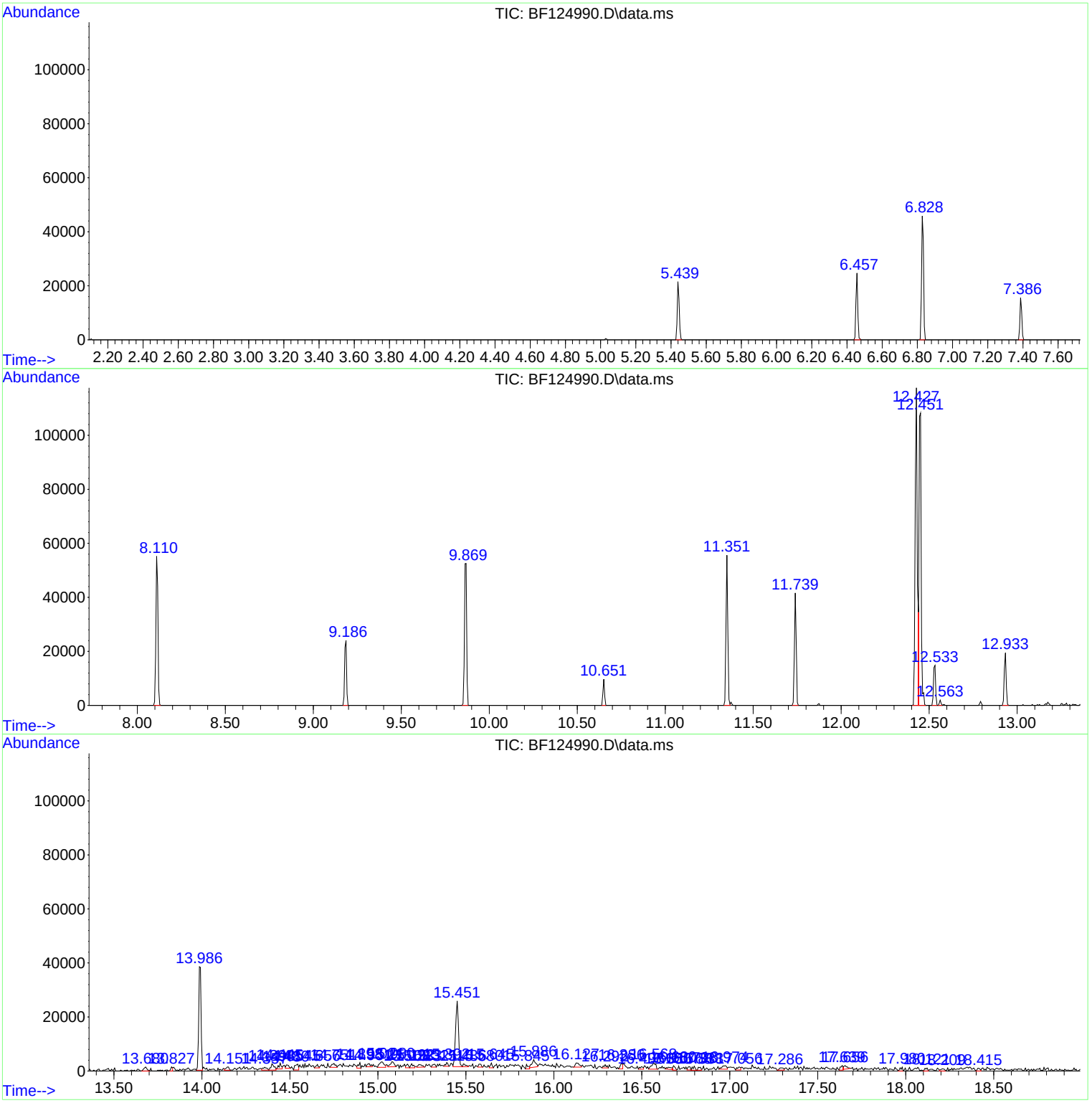
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-080521

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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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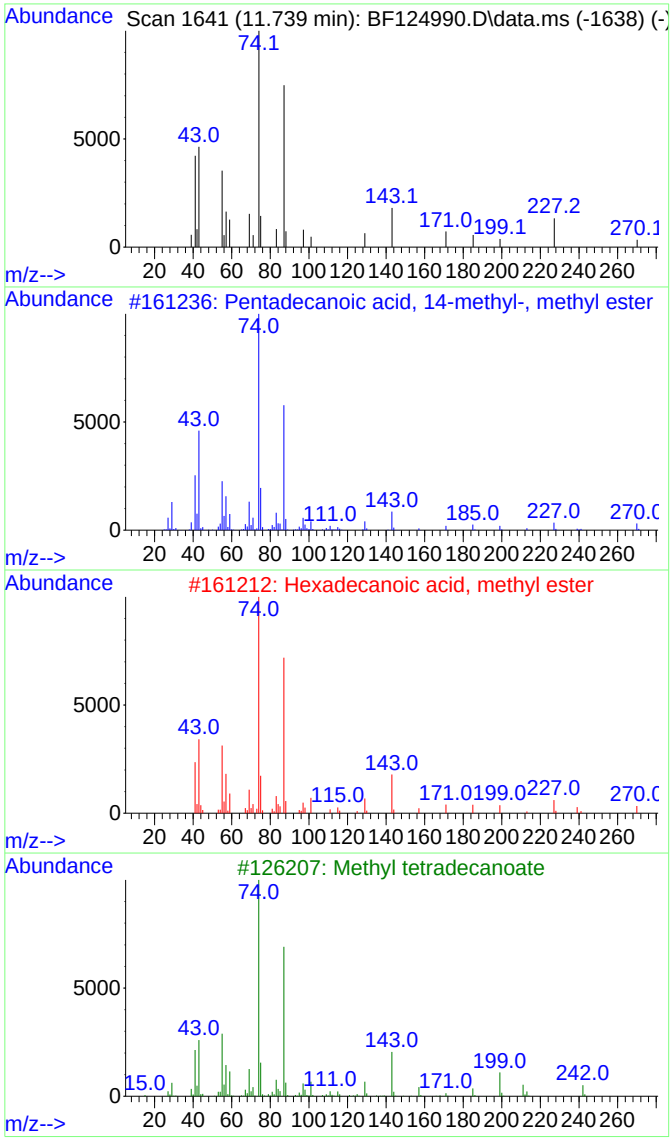
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

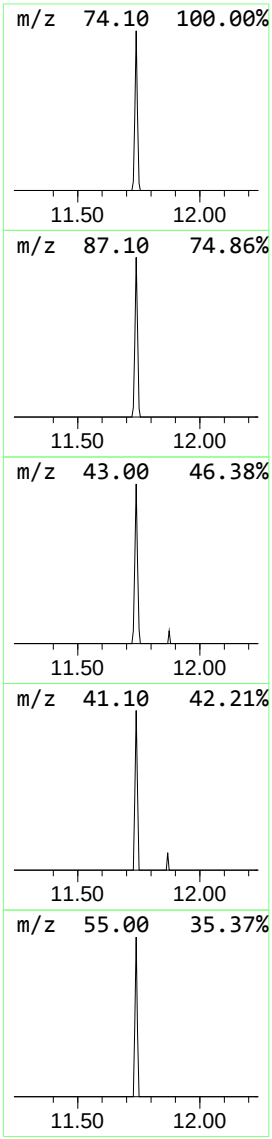
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentadecanoic acid, 14-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	14.91 ng	29575	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
2	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	94
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124990.D
Acq On : 8 Aug 2021 00:00
Operator : JU/CG
Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-080521

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

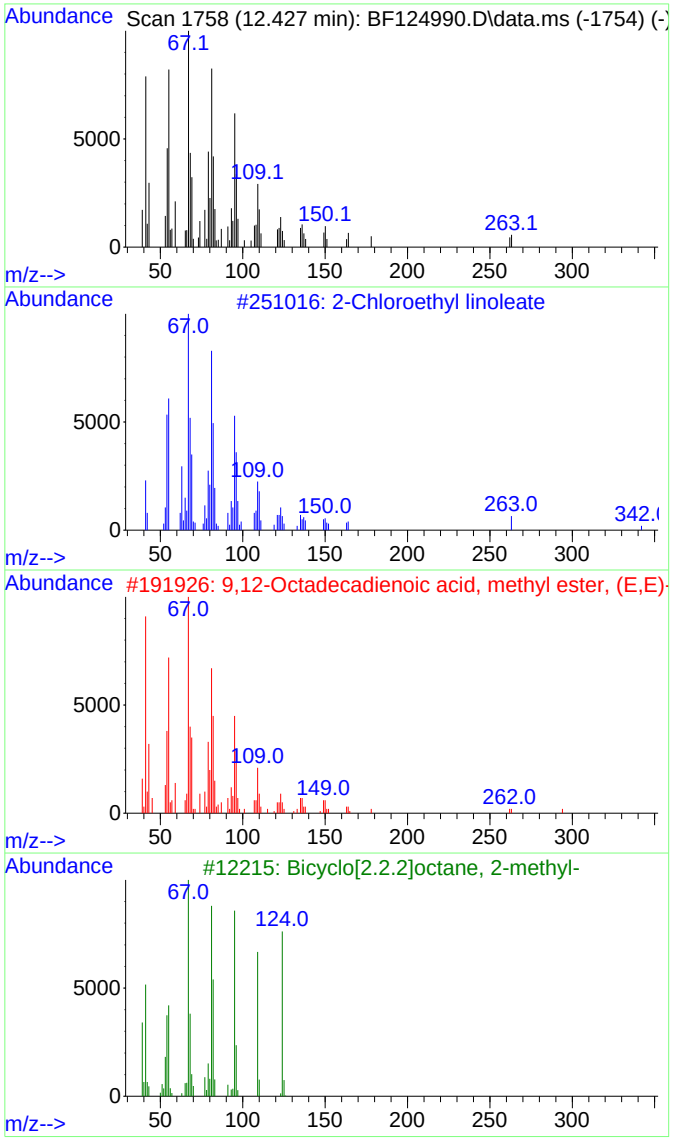
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

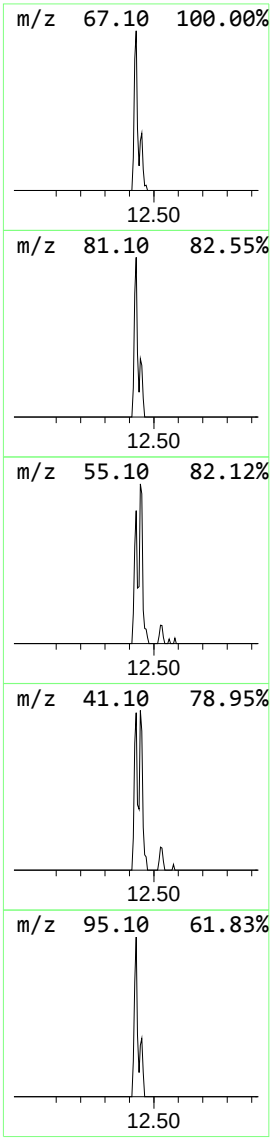
****

Peak Number 2 2-Chloroethyl linoleate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.427	53.09 ng	105301	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	76
3	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	74
4	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	74
5	11,14-Eicosadienoic acid, methyl...	322	C21H38O2	002463-02-7	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124990.D
Acq On : 8 Aug 2021 00:00
Operator : JU/CG
Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-080521

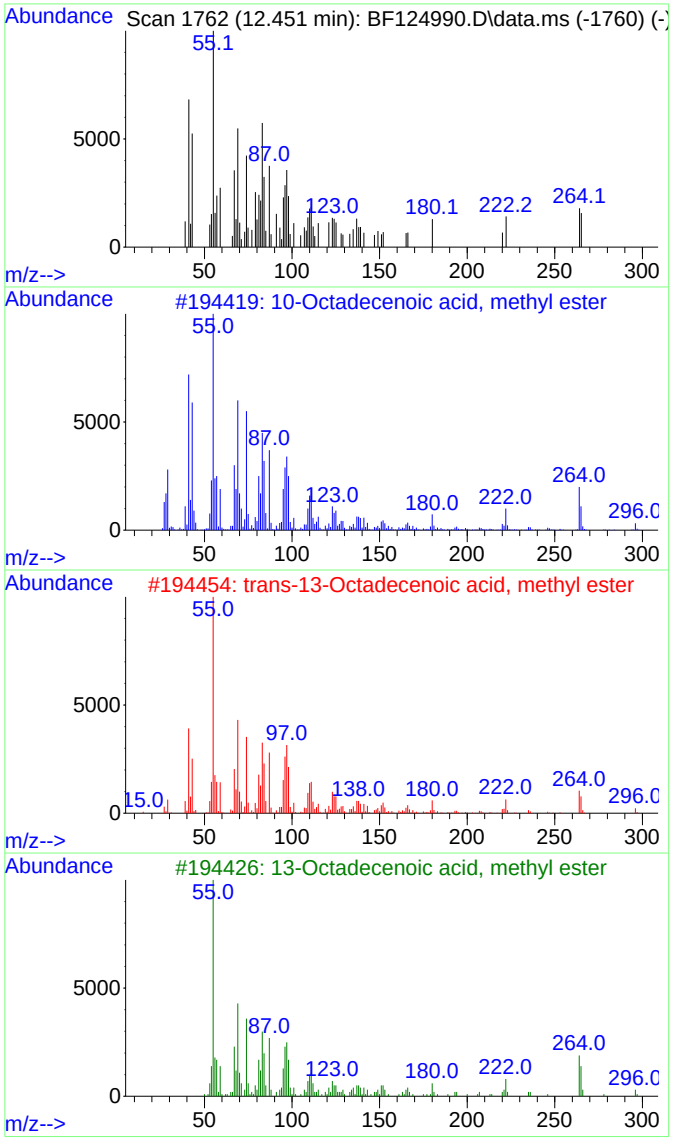
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

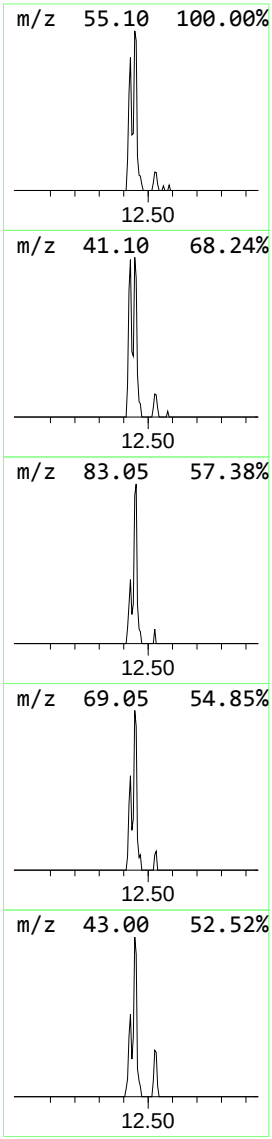
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 10-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	44.38 ng	88024	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	87
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	86
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	76
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124990.D
Acq On : 8 Aug 2021 00:00
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Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-080521

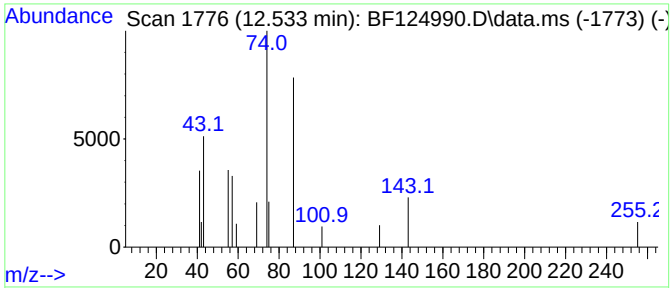
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

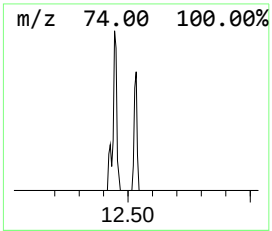
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

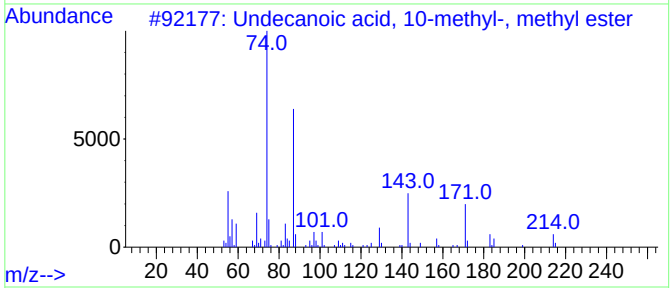
****
Peak Number 4 Undecanoic acid, 10-methyl-... Concentration Rank 4

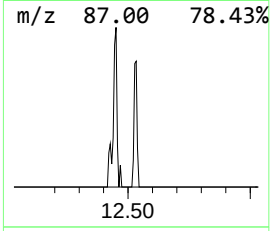
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	6.25 ng	12392	Phenanthrene-d10	11.351

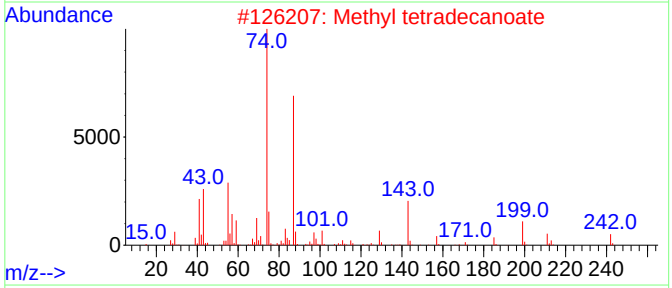
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid, 10-methyl-, met...	214	C13H26O2	005129-56-6	78
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	78
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	78
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	72
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72

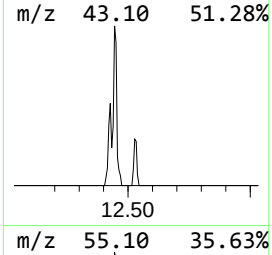


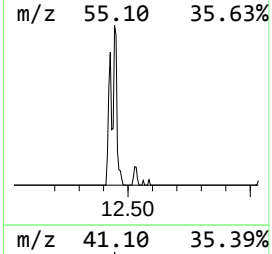


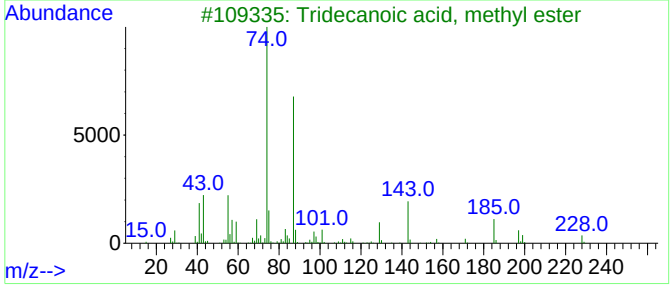


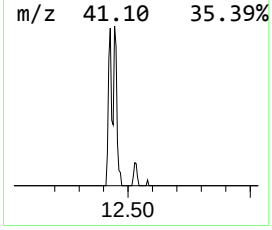












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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

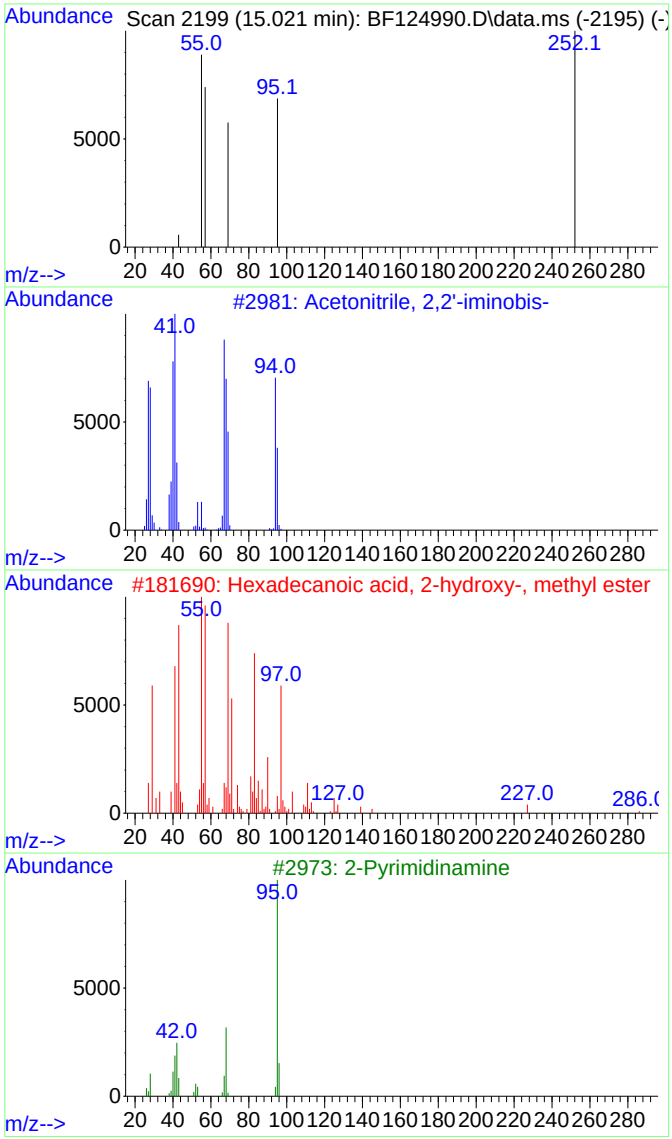
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

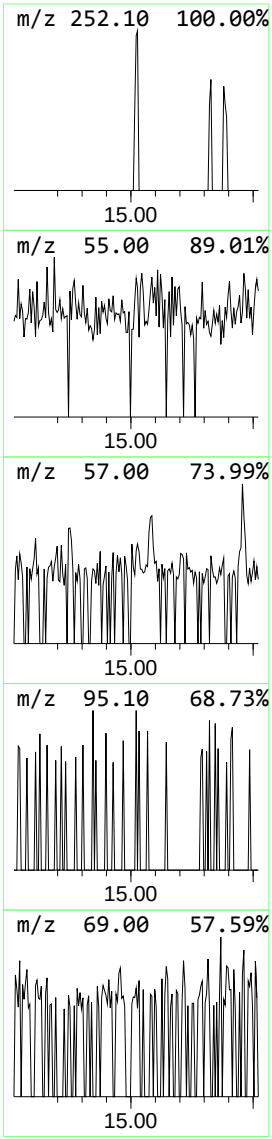
****

Peak Number 5 unknown15.021 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.021	2.75 ng	3846	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	4
2	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	4
3	2-Pyrimidinamine	95	C4H5N3	000109-12-6	3
4	3-Phenyl-4-anilino-4,5(1H)-dihyd...	252	C14H12N4O	057735-14-5	3
5	N-(3-Nitro-thiobenzoyl)-morpholine	252	C11H12N2O3S	050903-05-4	3





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Data File : BF124990.D
Acq On : 8 Aug 2021 00:00
Operator : JU/CG
Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-080521

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

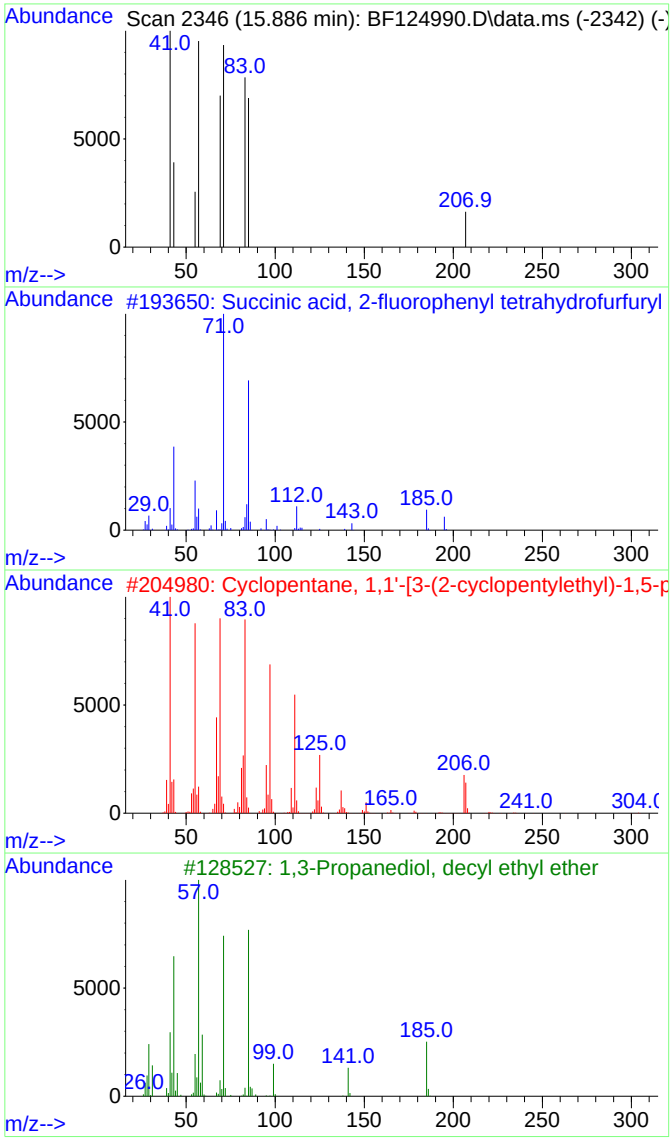
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

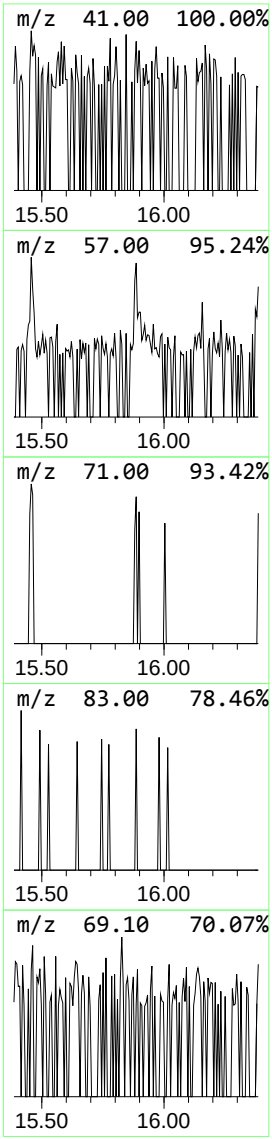
****

Peak Number 6 unknown15.886 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	2.98 ng	4169	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, 2-fluorophenyl te...	296	C15H17FO5	1000390-71-9	9
2	Cyclopentane, 1,1'-[3-(2-cyclope...	304	C22H40	055255-85-1	9
3	1,3-Propanediol, decyl ethyl ether	244	C15H32O2	1000406-35-0	9
4	Propane, 3,3-dichloro-1,1,1,2,2-...	202	C3HCl2F5	000422-56-0	9
5	Succinic acid, 2-chloro-6-fluoro...	330	C15H16ClFO5	1000390-72-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124990.D
Acq On : 8 Aug 2021 00:00
Operator : JU/CG
Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NB-08-080521

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

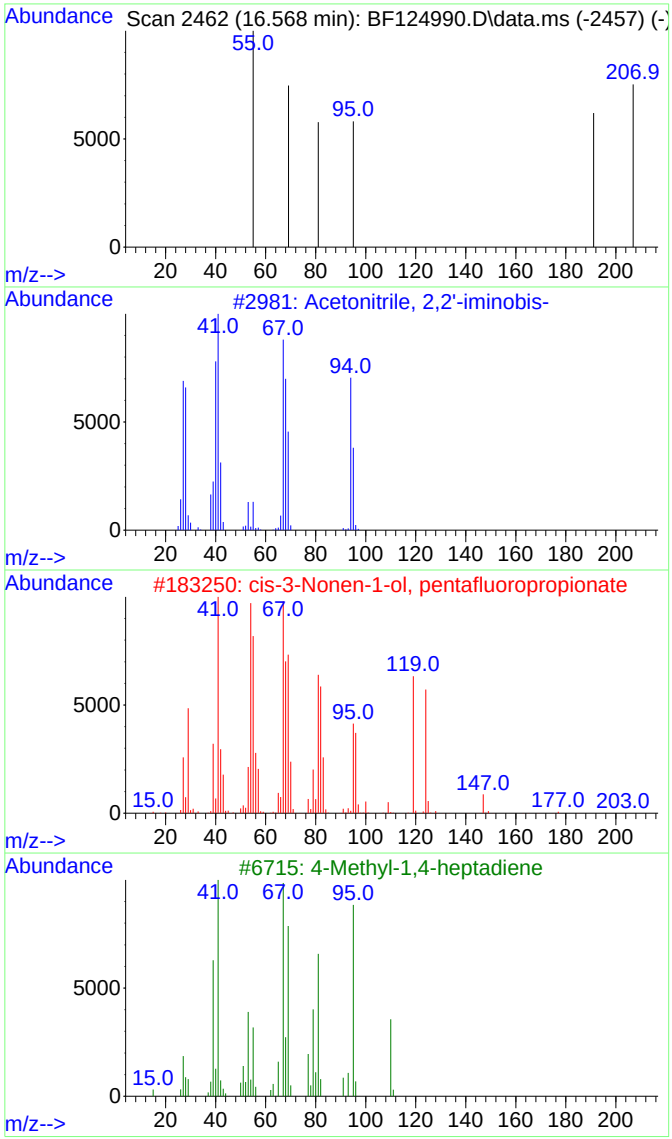
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

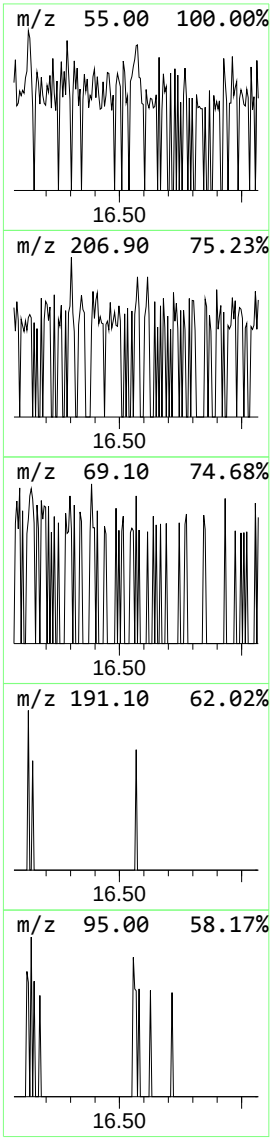
****

Peak Number 7 unknown16.568 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.568	2.84 ng	3967	Perylene-d12	15.451

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	4
2	cis-3-Nonen-1-ol, pentafluoropro...	288	C12H17F5O2	1000352-76-6	4
3	4-Methyl-1,4-heptadiene	110	C8H14	013857-55-1	4
4	Isopulegol	154	C10H18O	000089-79-2	4
5	Dithiocarbamate, S-methyl-,N-(2-...	191	C7H13NOS2	135923-14-7	3





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124990.D
Acq On : 8 Aug 2021 00:00
Operator : JU/CG
Sample : M3310-01 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-080521

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
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
Pentadecanoic a...	11.739	14.9	ng	29575	4	11.351	39668	20.0
2-Chloroethyl l...	12.427	53.1	ng	105301	4	11.351	39668	20.0
10-Octadecenoic...	12.451	44.4	ng	88024	4	11.351	39668	20.0
Undecanoic acid...	12.533	6.3	ng	12392	4	11.351	39668	20.0
unknown15.021	15.021	2.8	ng	3846	6	15.451	27980	20.0
unknown15.886	15.886	3.0	ng	4169	6	15.451	27980	20.0
unknown16.568	16.568	2.8	ng	3967	6	15.451	27980	20.0