LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012522\
Data File : BF126666.D
Acq On : 25 Jan 2022 16:29
Operator : CG/JU
Sample : N1228-03
Misc :
ALS Vial : 14 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
1245-N43502

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	27	34	40	rVB	1231255	1608172	49.38%	5.843%
2	5.187	524	527	532	rBV	41467	45023	1.38%	0.164%
3	5.575	589	593	597	rBV	1947361	1843093	56.60%	6.696%
4	5.910	647	650	656	rVB	56447	55069	1.69%	0.200%
5	6.446	737	741	744	rBV	43680	39657	1.22%	0.144%
6	6.522	750	754	758	rBV4	30854	43303	1.33%	0.157%
7	6.569	758	762	767	rBV	1476530	1329479	40.82%	4.830%
8	6.769	790	796	797	rBV2	135720	176460	5.42%	0.641%
9	6.875	808	814	822	rVB	148069	153296	4.71%	0.557%
10	6.963	825	829	832	rBV	1610045	1302520	40.00%	4.732%
11	7.016	834	838	842	rBV	199284	187473	5.76%	0.681%
12	7.140	855	859	862	rVB3	38047	48636	1.49%	0.177%
13	7.440	905	910	914	rBV4	36130	59095	1.81%	0.215%
14	7.522	919	924	927	rVV	2172128	2082887	63.96%	7.567%
15	7.616	931	940	942	rVV	230770	455310	13.98%	1.654%
16	7.669	945	949	951	rVB3	30407	40874	1.26%	0.149%
17	7.698	951	954	957	rBV2	61610	53291	1.64%	0.194%
18	7.804	970	972	977	rVB2	59830	59217	1.82%	0.215%
19	7.969	990	1000	1004	rVB2	250668	518801	15.93%	1.885%
20	8.145	1026	1030	1033	rBV2	58992	71679	2.20%	0.260%
21	8.245	1042	1047	1050	rBV	1924852	1729059	53.09%	6.282%
22	8.734	1127	1130	1132	rVB	104740	77612	2.38%	0.282%
23	8.798	1137	1141	1144	rBV3	28834	44941	1.38%	0.163%
24	8.834	1144	1147	1150	rVV3	49059	50756	1.56%	0.184%
25	8.869	1150	1153	1157	rVB4	32819	39575	1.22%	0.144%
26	8.975	1168	1171	1173	rBV	65260	59038	1.81%	0.214%
27	8.998	1173	1175	1180	rVB	42205	36861	1.13%	0.134%
28	9.087	1187	1190	1195	rVB7	38211	54795	1.68%	0.199%
29	9.169	1200	1204	1205	rBV4	42146	48559	1.49%	0.176%
30	9.192	1205	1208	1212	rVB2	69399	82781	2.54%	0.301%
31	9.322	1225	1230	1233	rBV	3747516	3256549	100.00%	11.831%
32	9.392	1240	1242	1244	rVB	62709	48708	1.50%	0.177%
33	9.428	1244	1248	1251	rBV4	40186	66387	2.04%	0.241%
34	9.563	1268	1271	1273	rBV4	35670	42506	1.31%	0.154%
35	9.687	1290	1292	1294	rVB	51146	38818	1.19%	0.141%
36	9.716	1294	1297	1298	rBV3	47013	45967	1.41%	0.167%

LSC Area Percent Report

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Acq On : 25 Jan 2022 16:29
Operator : CG/JU
Sample : N1228-03
Misc :
ALS Vial : 14 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
1245-N43502

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.745	1300	1302	1305	rVB3	77010	78547	2.41%	0.285%
38	9.810	1311	1313	1319	rVB5	74858	84452	2.59%	0.307%
39	9.869	1320	1323	1325	rBV3	38750	42737	1.31%	0.155%
40	10.004	1342	1346	1350	rVB	2035958	1767883	54.29%	6.423%
41	10.128	1364	1367	1369	rBV3	50218	51037	1.57%	0.185%
42	10.186	1375	1377	1382	rVB5	54694	62438	1.92%	0.227%
43	10.569	1440	1442	1444	rVB	74241	48583	1.49%	0.177%
44	10.622	1449	1451	1453	rBV	60105	45877	1.41%	0.167%
45	10.792	1476	1480	1484	rBV	1883912	1789722	54.96%	6.502%
46	10.933	1503	1504	1507	rVB	132761	102776	3.16%	0.373%
47	11.328	1569	1571	1573	rBV	69195	63455	1.95%	0.231%
48	11.445	1589	1591	1593	rVB	62859	42253	1.30%	0.154%
49	11.498	1596	1600	1603	rBV	1959976	1599311	49.11%	5.811%
50	12.010	1685	1687	1690	rBV	258817	196298	6.03%	0.713%
51	12.339	1741	1743	1746	rBV	105671	72498	2.23%	0.263%
52	12.798	1818	1821	1825	rBV2	120114	120377	3.70%	0.437%
53	13.086	1866	1870	1873	rBV	2814761	2388470	73.34%	8.678%
54	13.563	1949	1951	1954	rVB	80774	64249	1.97%	0.233%
55	13.727	1977	1979	1984	rVB	63810	55618	1.71%	0.202%
56	13.886	2003	2006	2008	rBV	48806	42130	1.29%	0.153%
57	13.980	2019	2022	2029	rBV	150163	190777	5.86%	0.693%
58	14.145	2046	2050	2054	rVB	1219962	1121848	34.45%	4.076%
59	14.651	2134	2136	2142	rVB	64776	72581	2.23%	0.264%
60	15.668	2304	2309	2320	rVB	861622	1206439	37.05%	4.383%
61	15.939	2351	2355	2364	rVB4	33392	65620	2.02%	0.238%
62	16.168	2390	2394	2400	rBV5	22410	47472	1.46%	0.172%
63	16.427	2435	2438	2445	rVB7	24759	50929	1.56%	0.185%
64	16.715	2483	2487	2494	rVB6	26915	54308	1.67%	0.197%
65	16.892	2513	2517	2523	rVB6	33380	58697	1.80%	0.213%
66	17.433	2605	2609	2615	rVB9	23616	40821	1.25%	0.148%

Sum of corrected areas: 27524450

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Misc :
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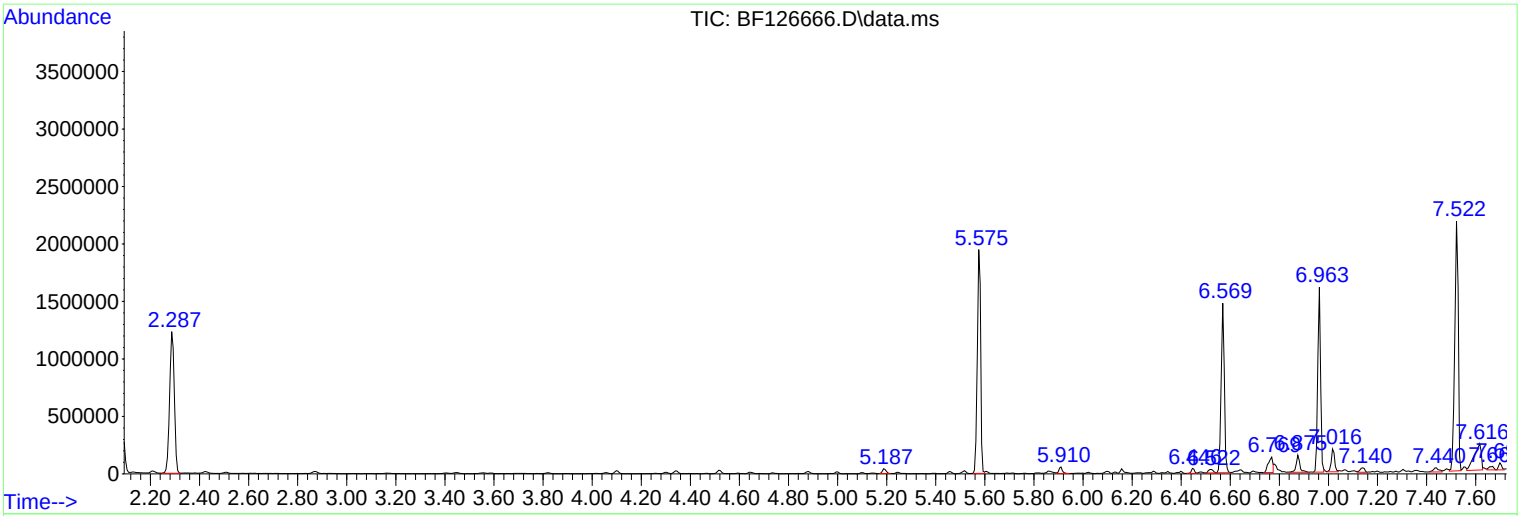
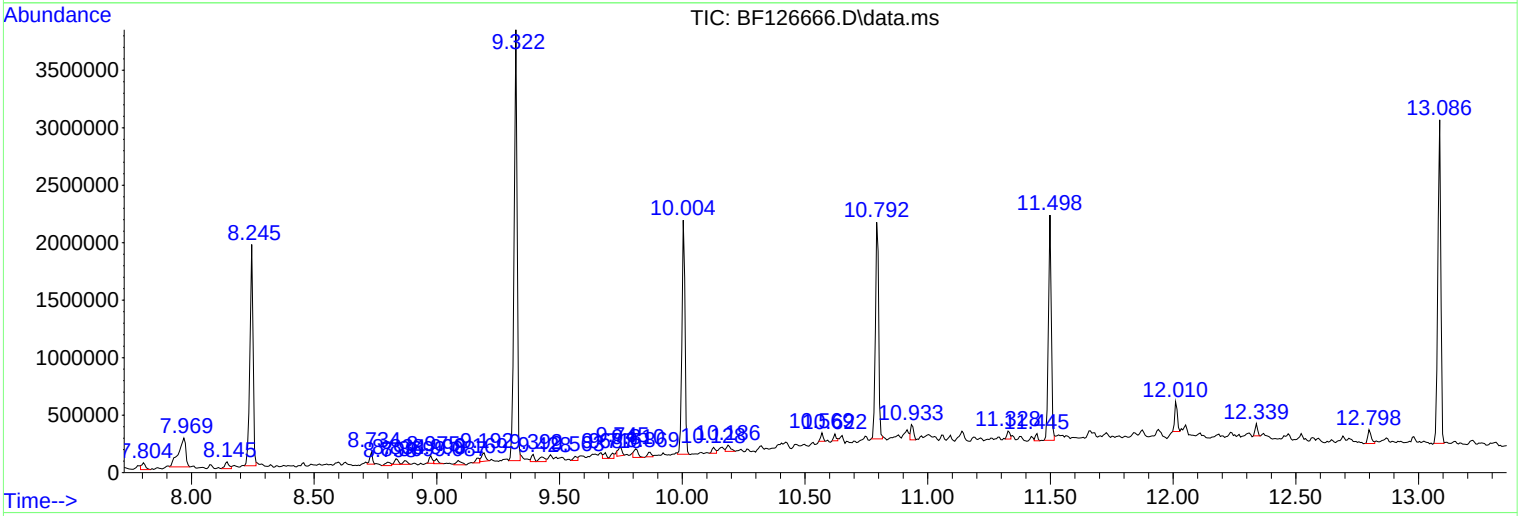
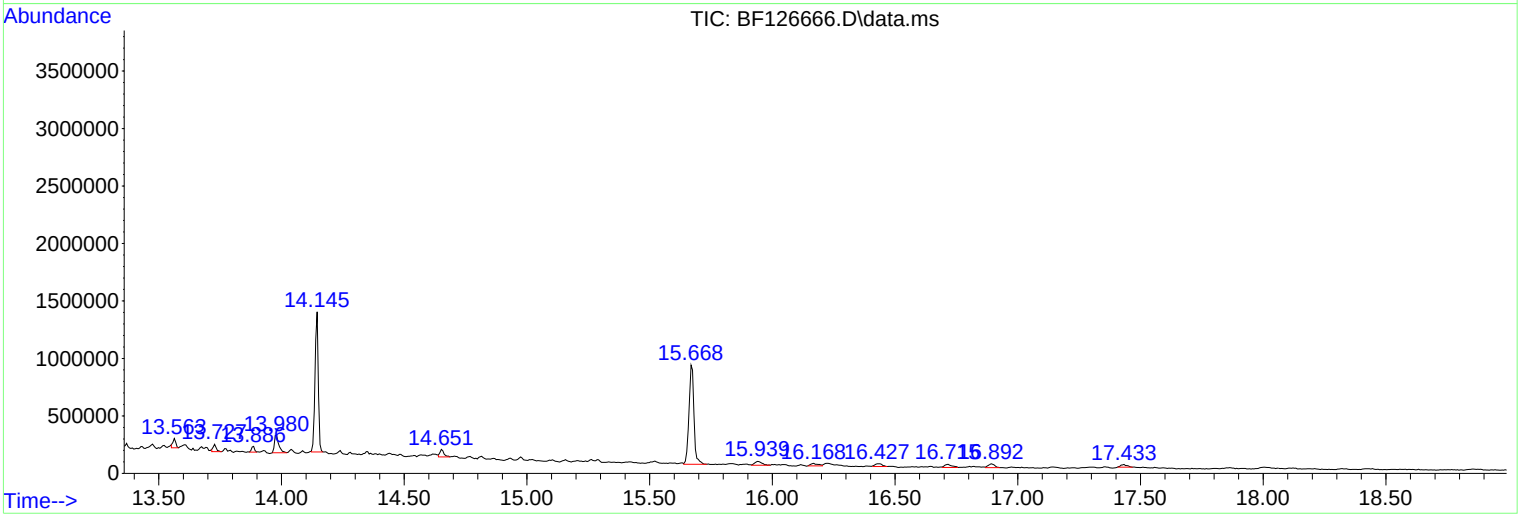
Instrument :
BNA_F
ClientSampleId :
1245-N43502

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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Instrument :
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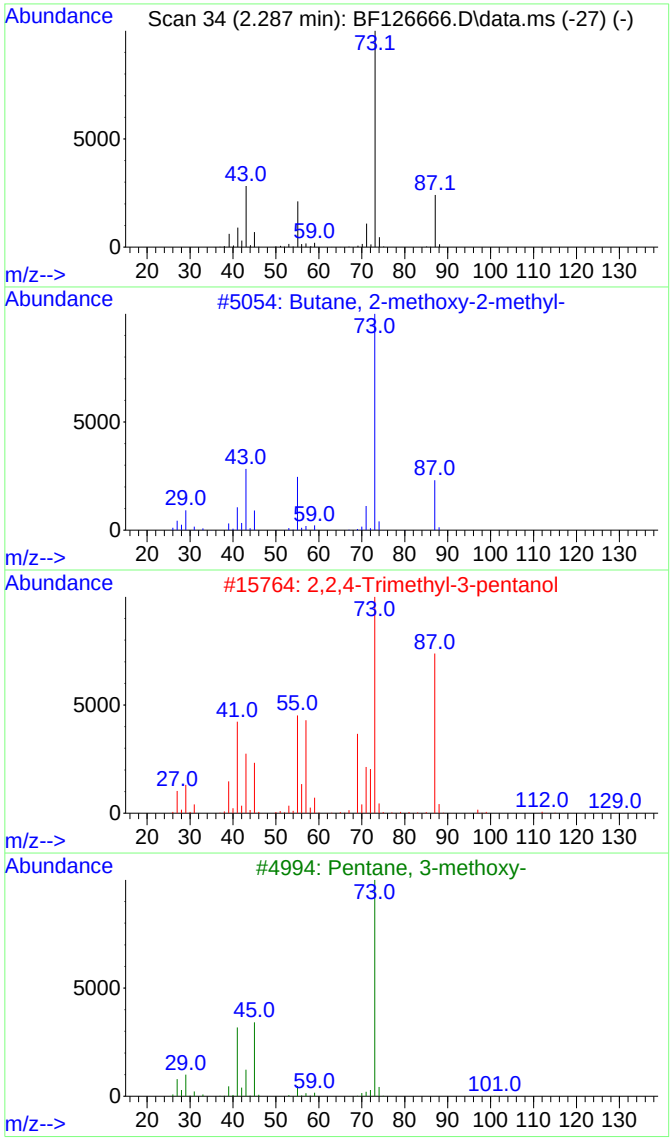
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

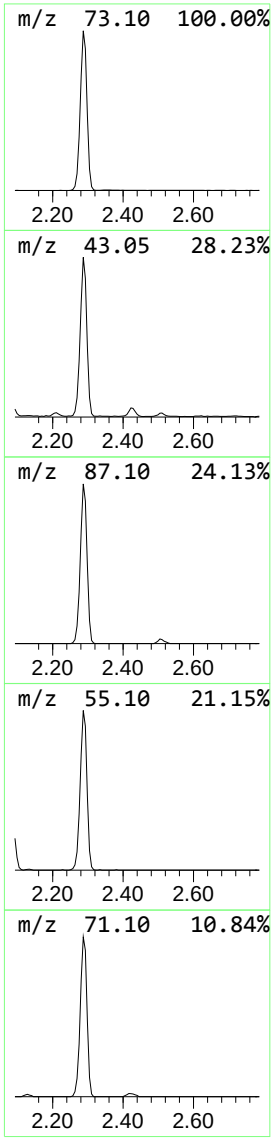
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	24.69 ng	1608170	1,4-Dichlorobenzene-d4	6.963

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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





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Operator : CG/JU
Sample : N1228-03
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

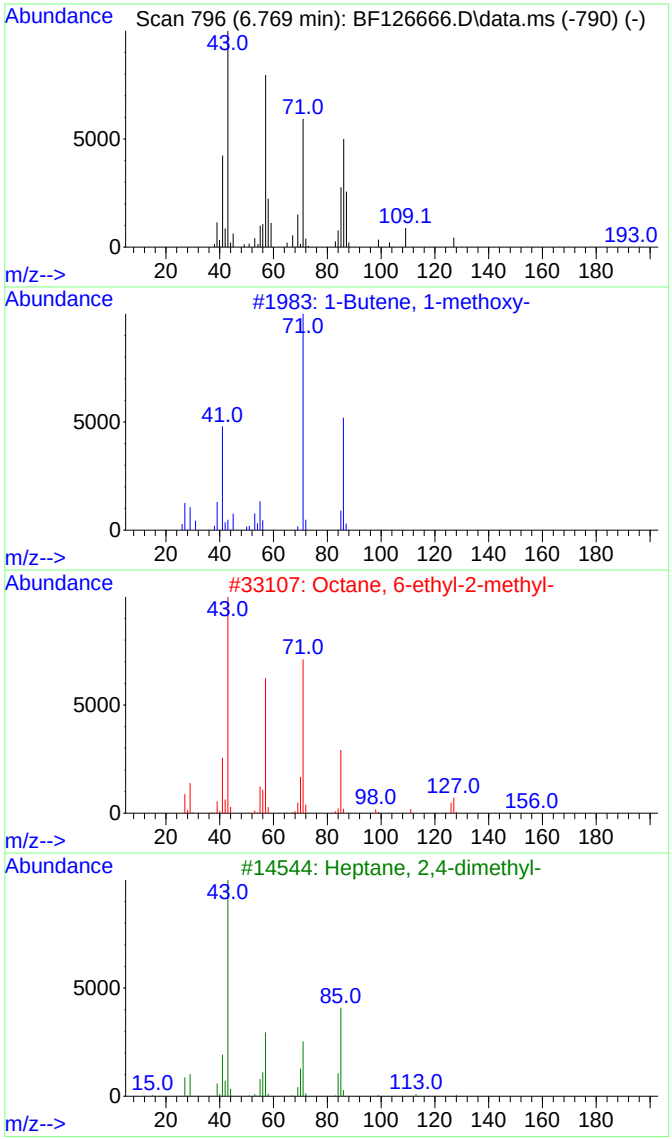
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

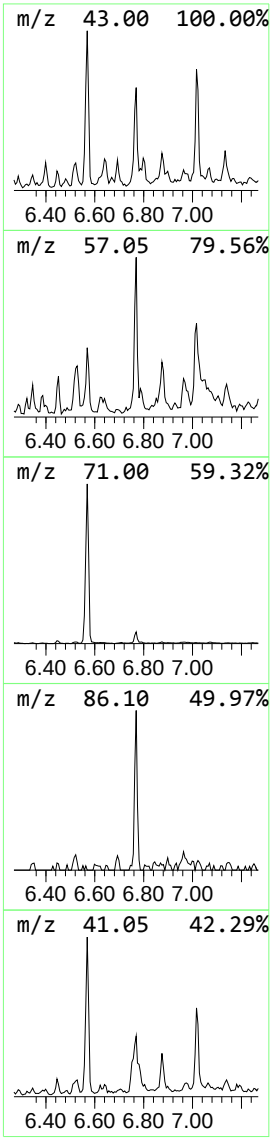
****

Peak Number 2 unknown6.769 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.769	2.71 ng	176460	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 1-methoxy-	86	C5H10O	029512-02-5	38
2	Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	35
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	35
4	Nonadecane	268	C19H40	000629-92-5	35
5	Carbonic acid, nonyl vinyl ester	214	C12H22O3	1000383-25-6	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012522\
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Instrument :
BNA_F
ClientSampleId :
1245-N43502

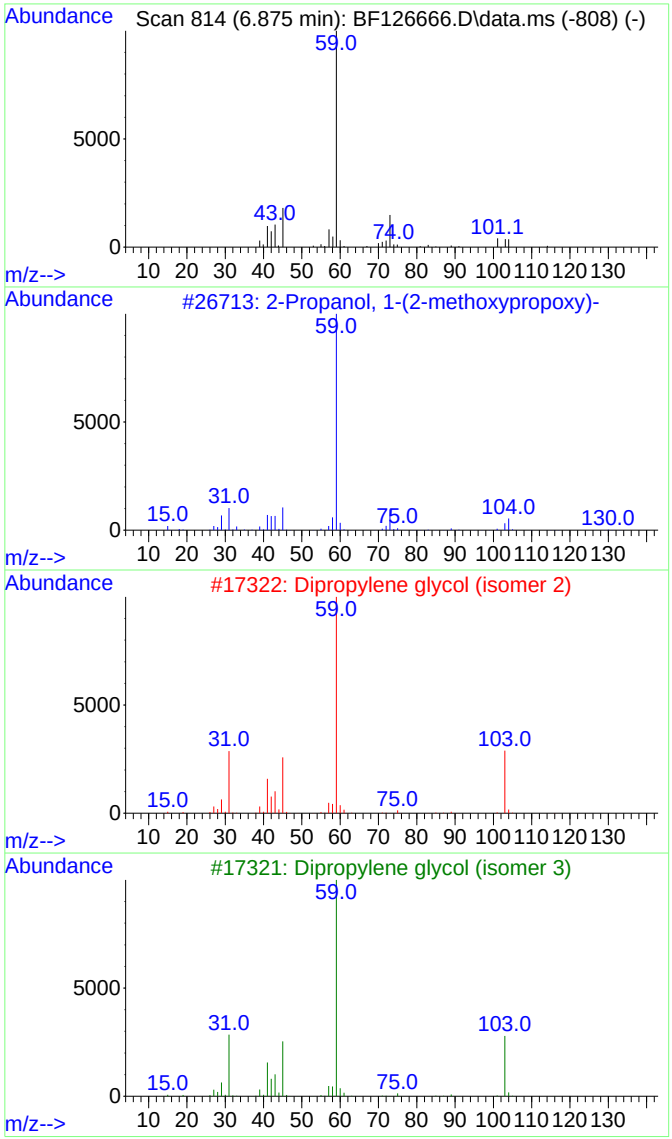
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

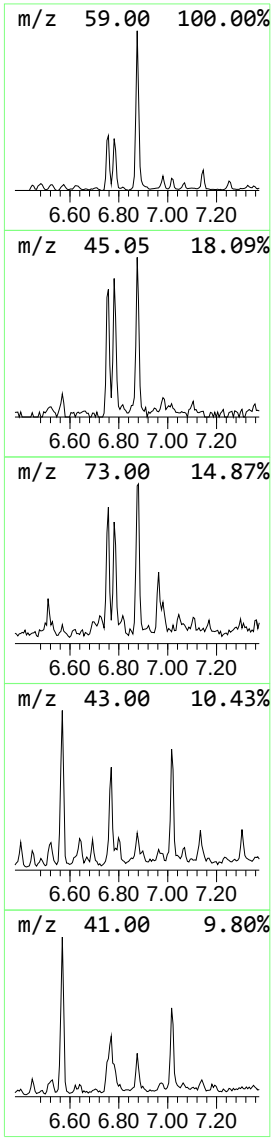
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxypro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.875	2.35 ng	153296	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	78
2	Dipropylene glycol (isomer 2)	134	C6H14O3	1000506-25-4	64
3	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	59
5	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	56





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

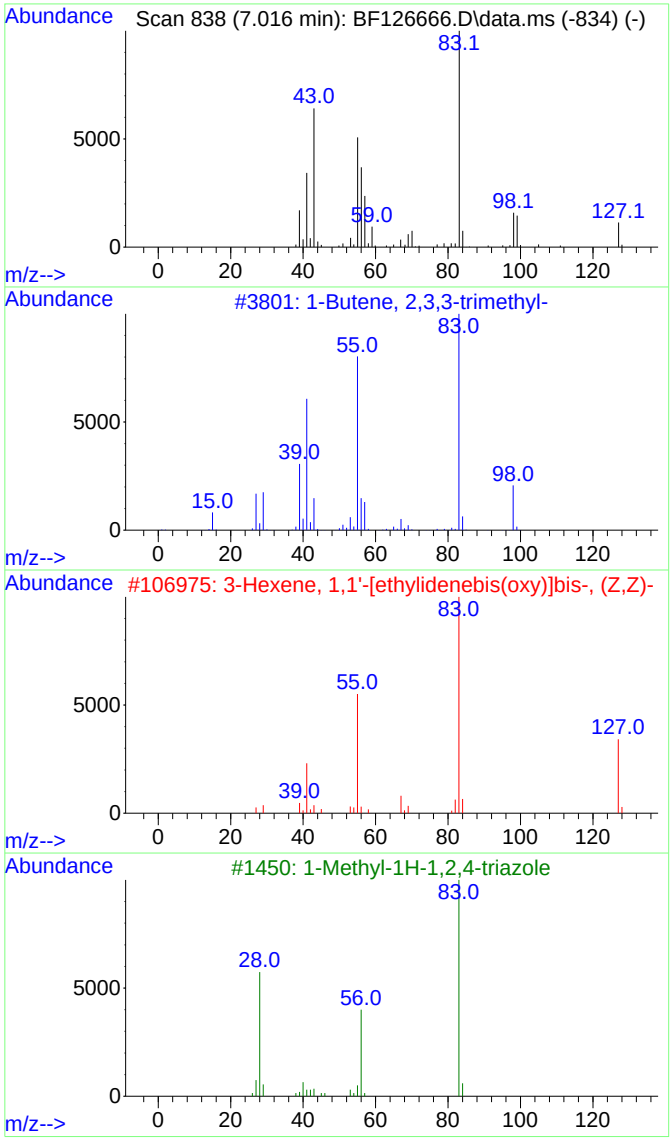
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

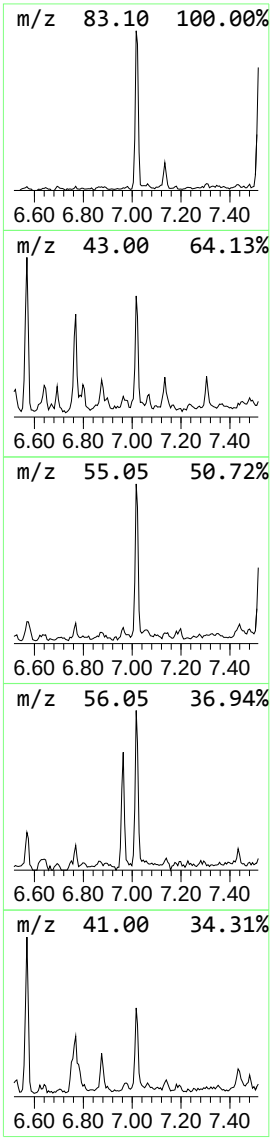
****

Peak Number 4 1-Butene, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.016	2.88 ng	187473	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	53
2	3-Hexene, 1,1'-[ethylidenebis(ox...	226	C14H26O2	063449-64-9	50
3	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	50
4	Propanedinitrile, dicyclohexyl-	230	C15H22N2	074764-28-6	47
5	1,5-Heptadien-4-one, 3,3,6-trime...	152	C10H16O	000546-49-6	47





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ALS Vial : 14 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

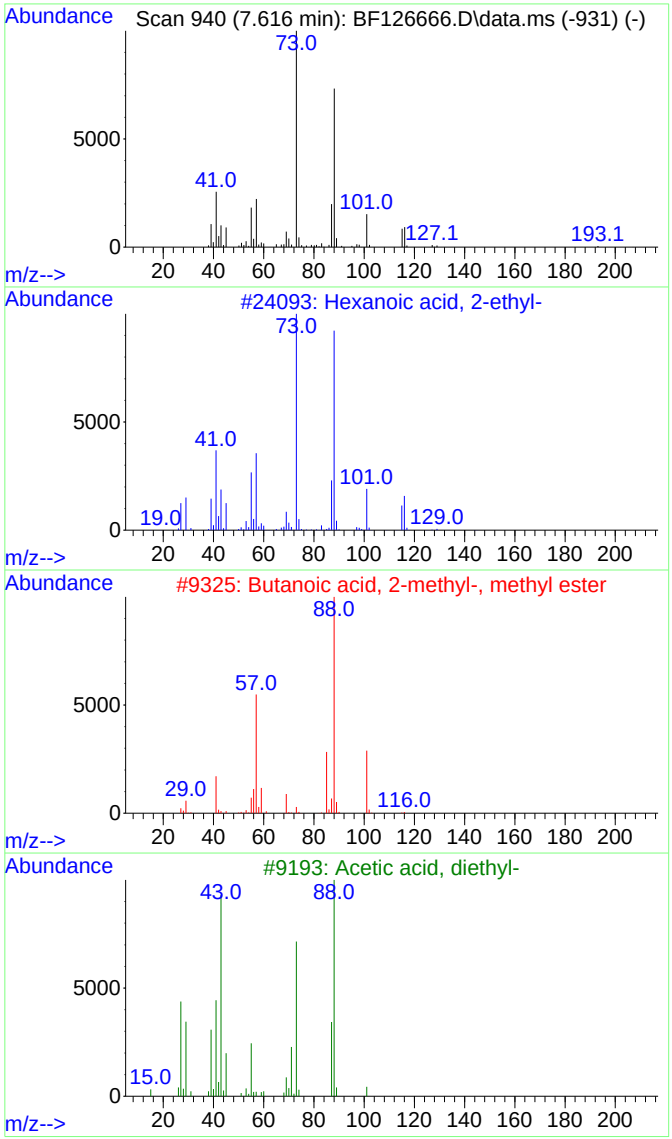
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

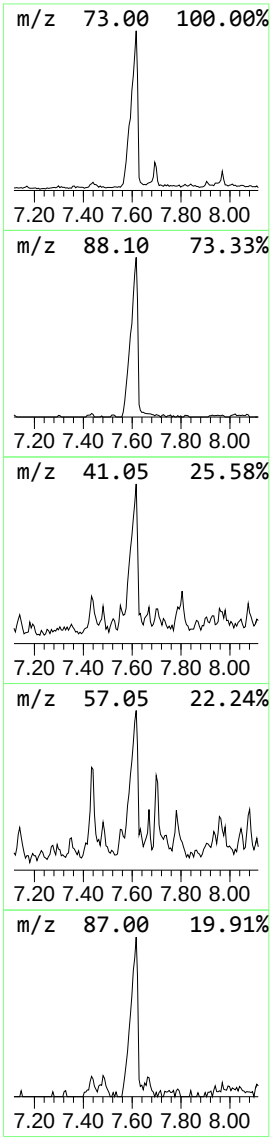
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.616	5.27 ng	455310	Naphthalene-d8	8.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47
3	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	45
4	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	45
5	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	45





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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

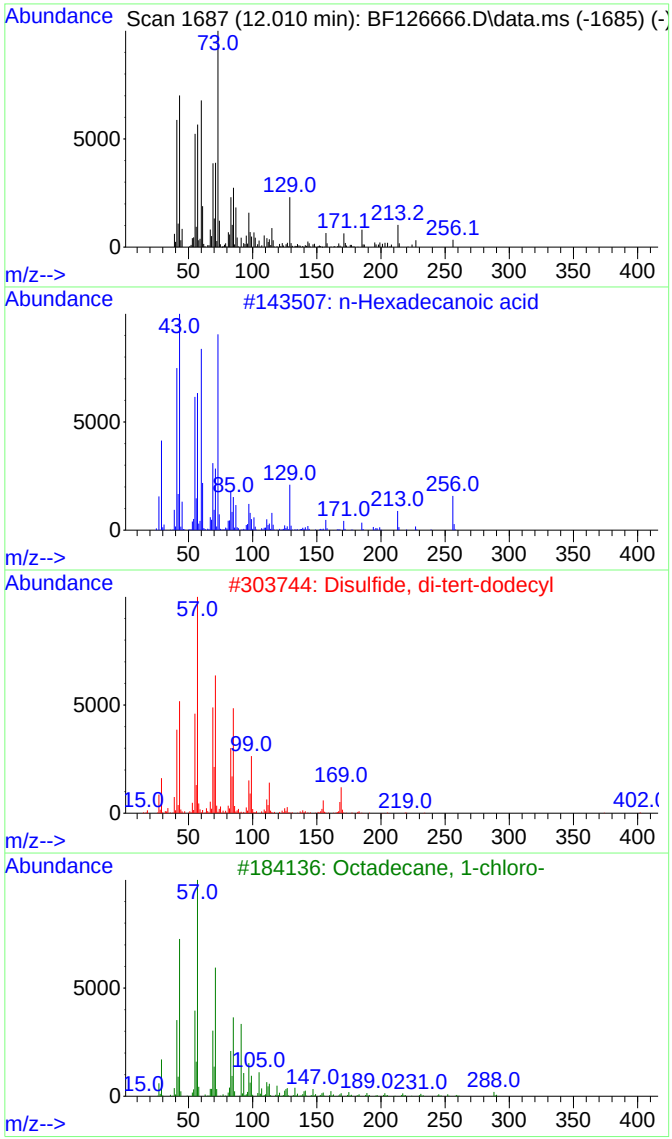
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

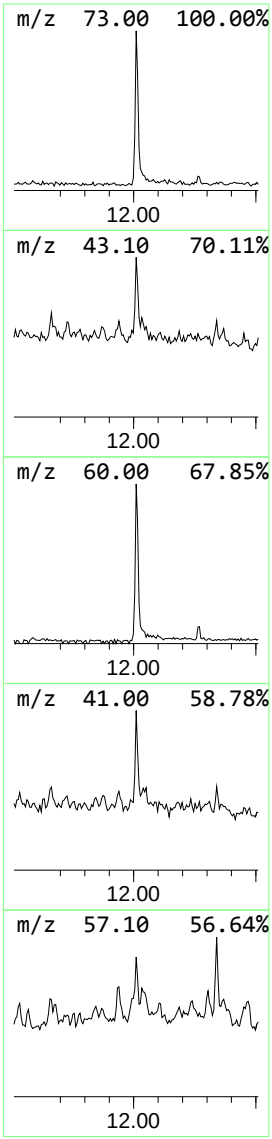
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	2.45 ng	196298	Phenanthrene-d10	11.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
2	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	45
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	38
4	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	38
5	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012522\
Data File : BF126666.D
Acq On : 25 Jan 2022 16:29
Operator : CG/JU
Sample : N1228-03
Misc :
ALS Vial : 14 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
1245-N43502

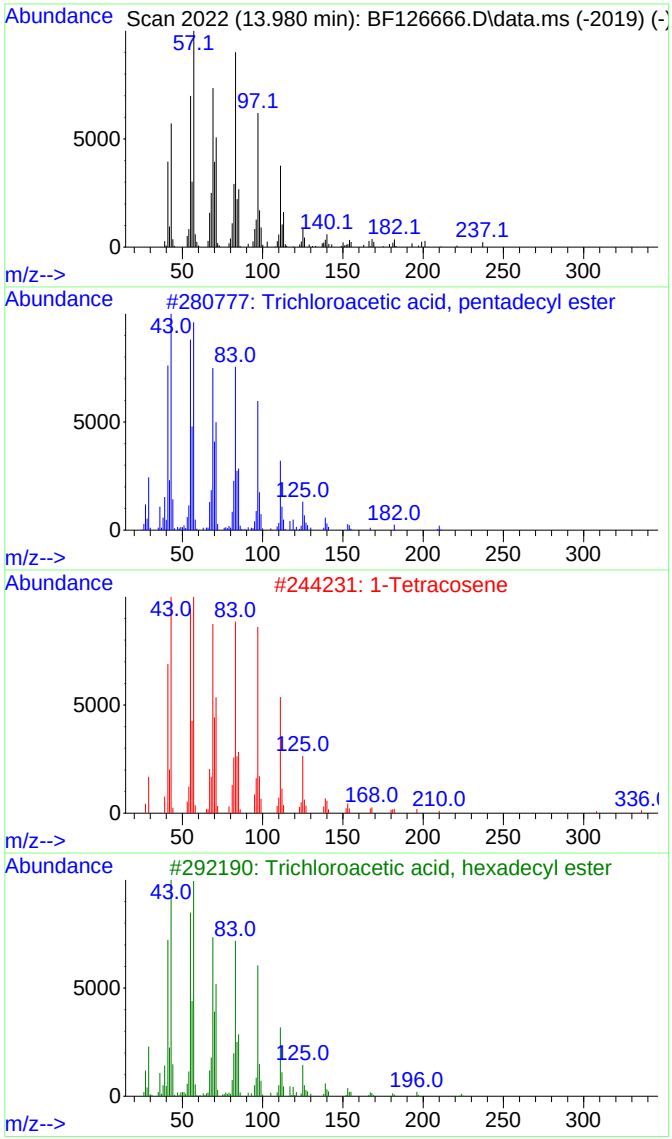
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

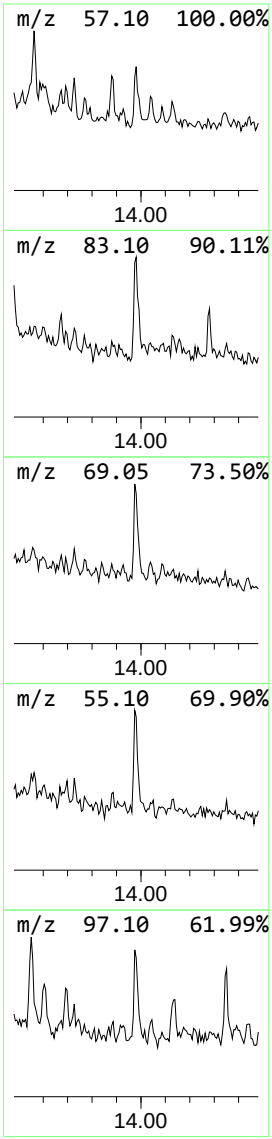
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	3.40 ng	190777	Chrysene-d12	14.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	1-Tetracosene	336	C24H48	010192-32-2	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012522\
Data File : BF126666.D
Acq On : 25 Jan 2022 16:29
Operator : CG/JU
Sample : N1228-03
Misc :
ALS Vial : 14 Sample Multiplier: 2

Instrument :
BNA_F
ClientSampleId :
1245-N43502

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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
Butane, 2-metho...	2.287	24.7	ng	1608170	1	6.963	1302520	20.0
unknown6.769	6.769	2.7	ng	176460	1	6.963	1302520	20.0
2-Propanol, 1-(...	6.875	2.4	ng	153296	1	6.963	1302520	20.0
1-Butene, 2,3,3...	7.016	2.9	ng	187473	1	6.963	1302520	20.0
Hexanoic acid, ...	7.616	5.3	ng	455310	2	8.245	1729060	20.0
n-Hexadecanoic ...	12.010	2.5	ng	196298	4	11.498	1599310	20.0
Trichloroacetic...	13.980	3.4	ng	190777	5	14.145	1121850	20.0