LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PSC-124037

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_G\Methods\8270-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054912.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.200	318	325	334	rBV	58991	92485	4.30%	0.667%
2	5.682	400	407	420	rBV	546657	888811	41.31%	6.408%
3	7.298	674	682	699	rBV	534648	939906	43.69%	6.776%
4	8.138	818	825	834	rBV	111531	191652	8.91%	1.382%
5	9.313	1017	1025	1041	rBV	316386	589134	27.38%	4.248%
6	10.717	1258	1264	1280	rBV	34668	83610	3.89%	0.603%
7	10.970	1298	1307	1313	rBV	151679	285903	13.29%	2.061%
8	13.397	1713	1720	1736	rBV	916182	1435983	66.75%	10.353%
9	14.777	1940	1955	1961	rBV	283213	449371	20.89%	3.240%
10	15.823	2126	2133	2139	rBV	22216	35660	1.66%	0.257%
11	16.264	2202	2208	2221	rBV	731550	1176732	54.69%	8.484%
12	16.464	2237	2242	2248	rBV6	12510	26059	1.21%	0.188%
13	17.521	2416	2422	2427	rBV	354882	583286	27.11%	4.205%
14	17.568	2427	2430	2436	rVB	68753	95865	4.46%	0.691%
15	17.656	2439	2445	2451	rBV	111648	175937	8.18%	1.268%
16	18.449	2577	2580	2584	rVB2	21119	26952	1.25%	0.194%
17	18.526	2590	2593	2598	rVB	21763	30027	1.40%	0.216%
18	18.596	2600	2605	2609	rBV3	38007	65233	3.03%	0.470%
19	18.896	2652	2656	2661	rBV	15113	21764	1.01%	0.157%
20	19.301	2722	2725	2730	rBV3	19568	25427	1.18%	0.183%
21	19.454	2747	2751	2760	rVB	38399	69056	3.21%	0.498%
22	19.572	2766	2771	2776	rBV	276746	385032	17.90%	2.776%
23	19.901	2823	2827	2828	rBV	45985	54863	2.55%	0.396%
24	19.936	2829	2833	2841	rVB	288386	421688	19.60%	3.040%
25	20.124	2859	2865	2870	rBV	1611715	2151445	100.00%	15.511%
26	20.247	2882	2886	2887	rBV3	22460	27731	1.29%	0.200%
27	20.523	2928	2933	2936	rBV	52785	74603	3.47%	0.538%
28	20.582	2941	2943	2947	rVB	38410	42615	1.98%	0.307%
29	20.723	2963	2967	2971	rBV	31426	38845	1.81%	0.280%
30	20.770	2972	2975	2979	rVB2	22896	29116	1.35%	0.210%
31	20.899	2995	2997	3001	rVB	19501	21515	1.00%	0.155%
32	21.193	3044	3047	3056	rVB	23713	39553	1.84%	0.285%
33	21.422	3082	3086	3092	rVV3	51081	95896	4.46%	0.691%
34	21.475	3092	3095	3101	rVB2	29419	46468	2.16%	0.335%
35	21.816	3144	3153	3158	rBV2	416226	936273	43.52%	6.750%
36	21.863	3158	3161	3174	rVB	184766	329089	15.30%	2.373%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

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_G\Methods\8270-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.022	3184	3188	3198	rVB4	26744	62285	2.90%	0.449%
38	22.239	3220	3225	3230	rVB2	13274	27160	1.26%	0.196%
39	23.338	3408	3412	3424	rVB9	18979	53797	2.50%	0.388%
40	23.549	3442	3448	3459	rVB	67913	154966	7.20%	1.117%
41	24.113	3536	3544	3552	rBV2	90073	300496	13.97%	2.167%
42	24.384	3586	3590	3599	rVB	14752	35422	1.65%	0.255%
43	24.871	3665	3673	3689	rVB2	55752	181162	8.42%	1.306%
44	25.030	3691	3700	3713	rVB	69266	212865	9.89%	1.535%
45	25.194	3715	3728	3737	rBV2	235843	743397	34.55%	5.360%
46	29.072	4382	4388	4408	rVB3	23977	114974	5.34%	0.829%

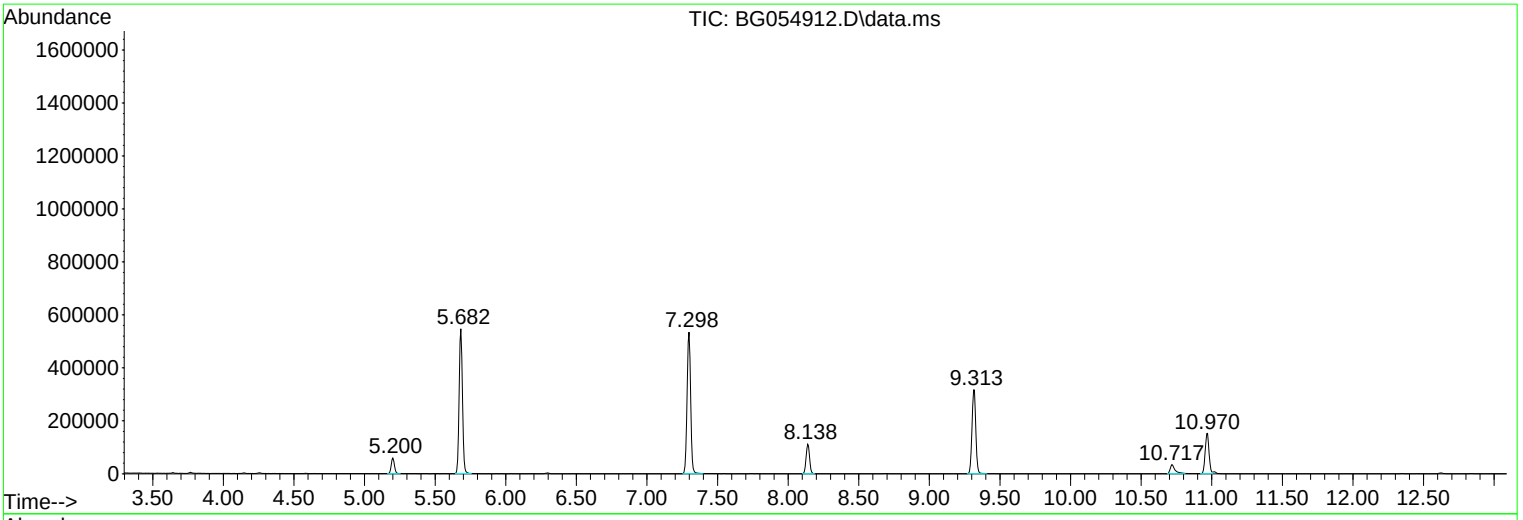
Sum of corrected areas: 13870109

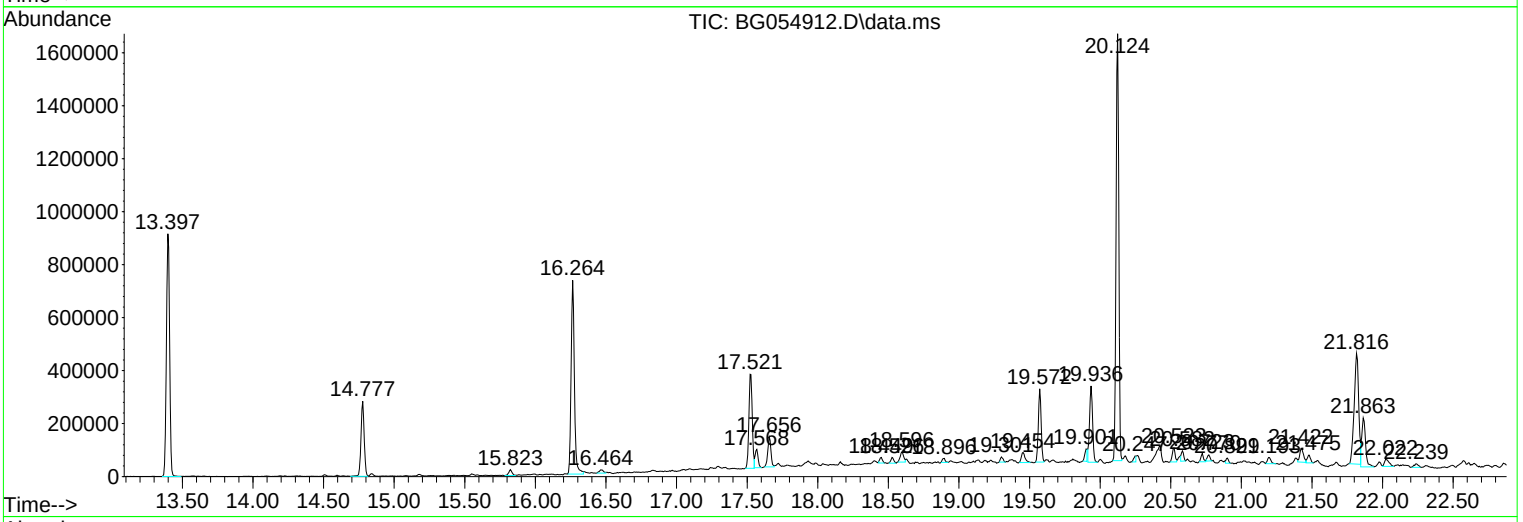
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

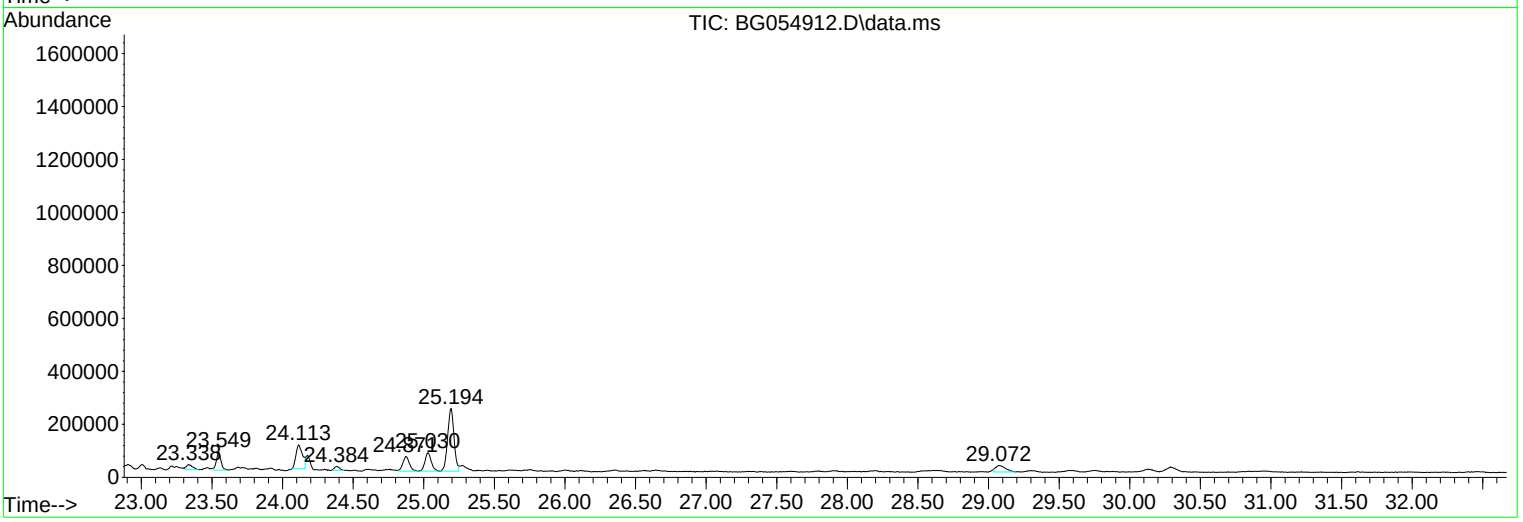
Instrument :
BNA_G
ClientSampleId :
PSC-124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

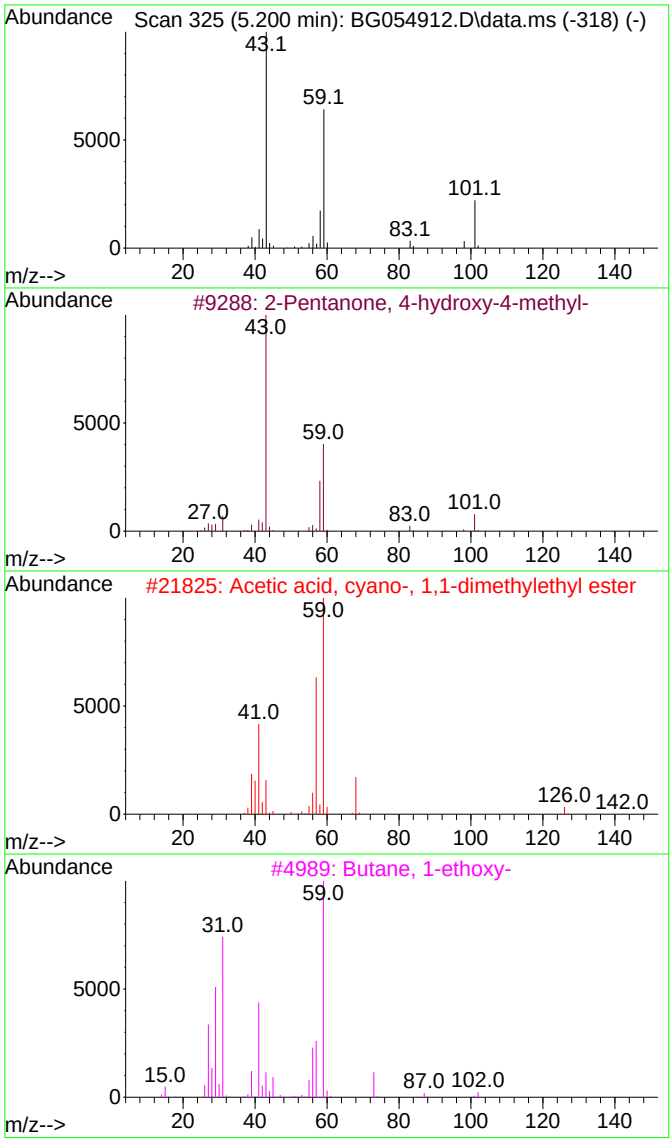
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

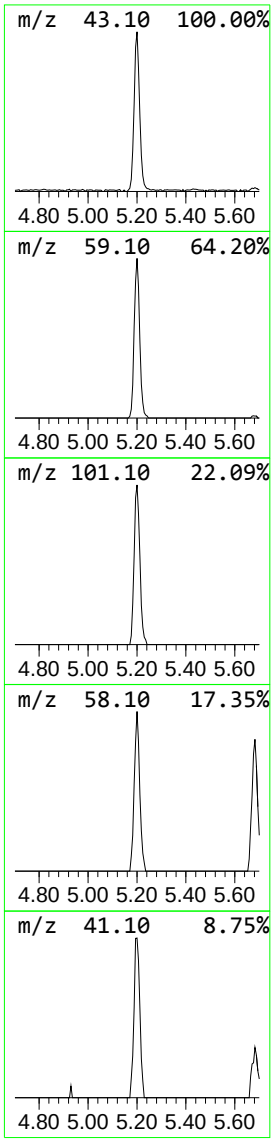
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.200	9.65 ng	92485	1,4-Dichlorobenzene-d4	8.138

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

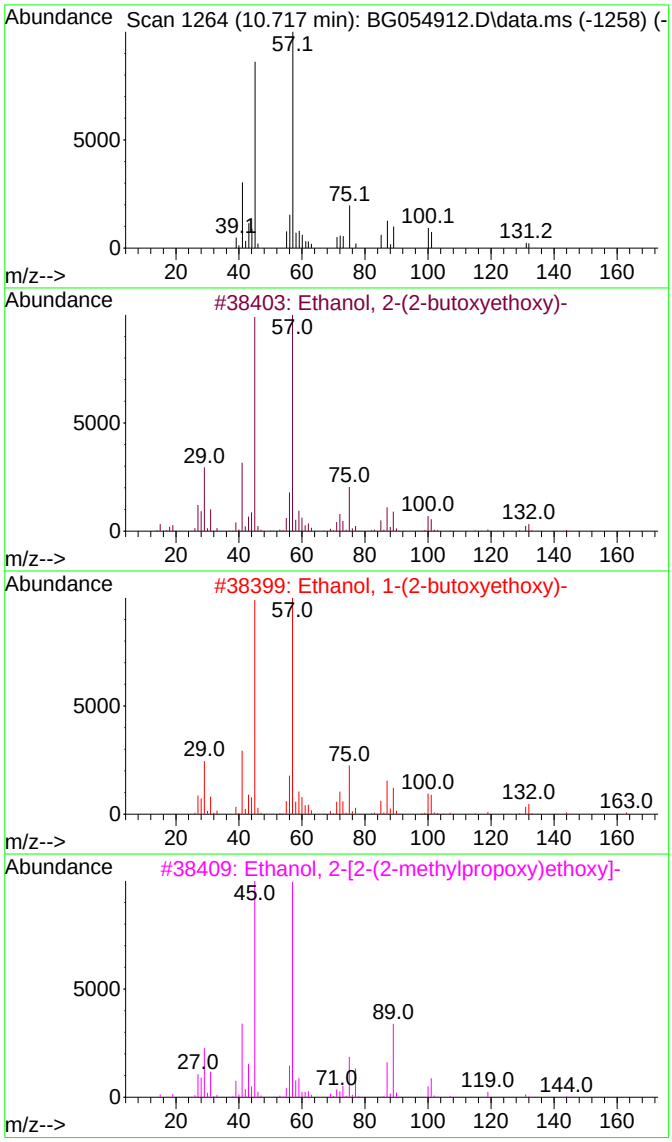
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

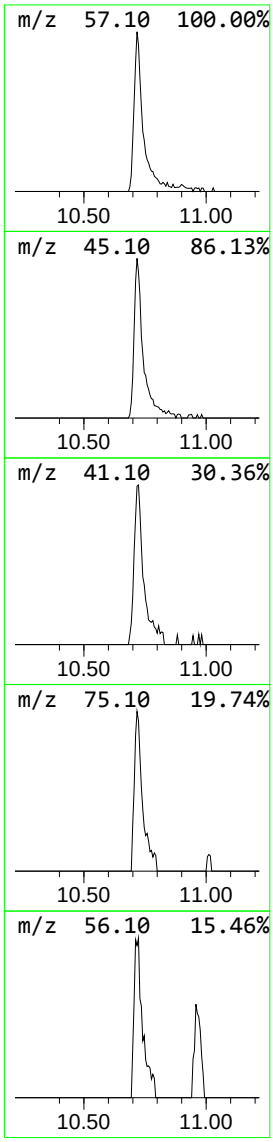
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.717	5.85 ng	83610	Naphthalene-d8	10.970

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

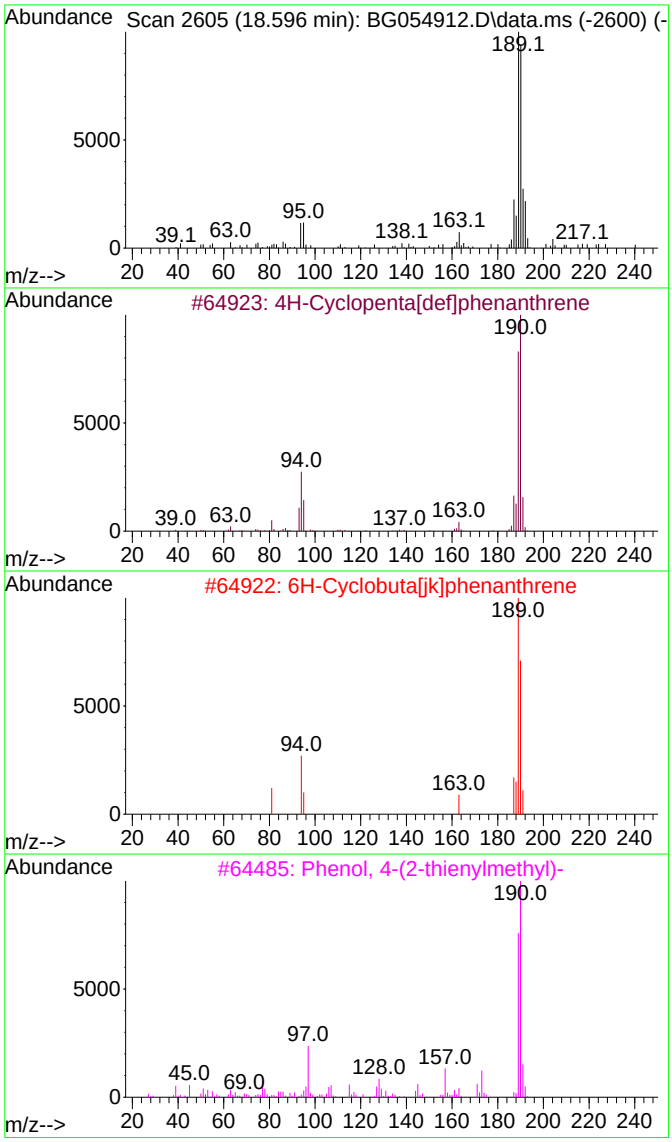
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

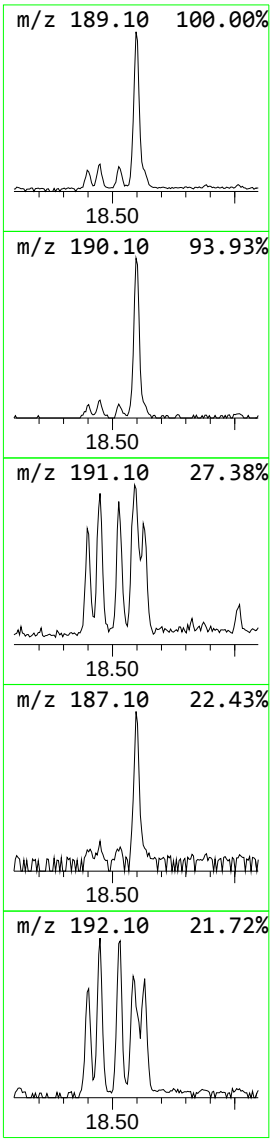
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.596	2.24 ng	65233	Phenanthrene-d10	17.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	40
4	Pyrimidine, 2-chloro-5-phenyl-	190	C10H7ClN2	022536-62-5	25
5	Cyclohexanone, 2-(2-furanylmethy...	190	C12H14O2	056053-07-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

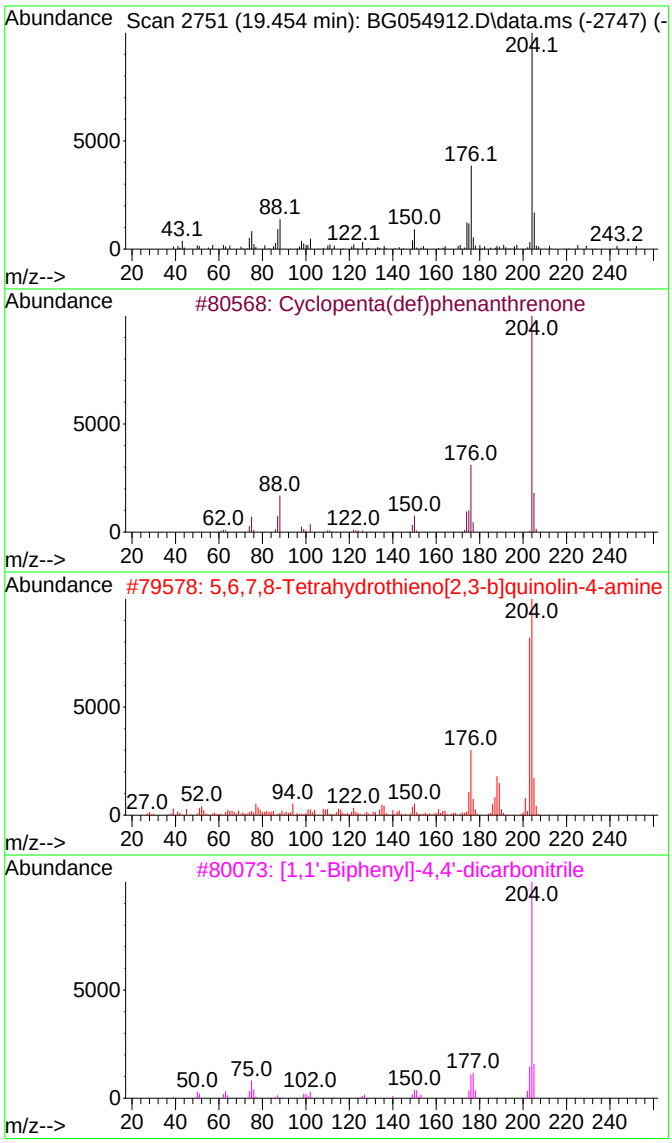
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

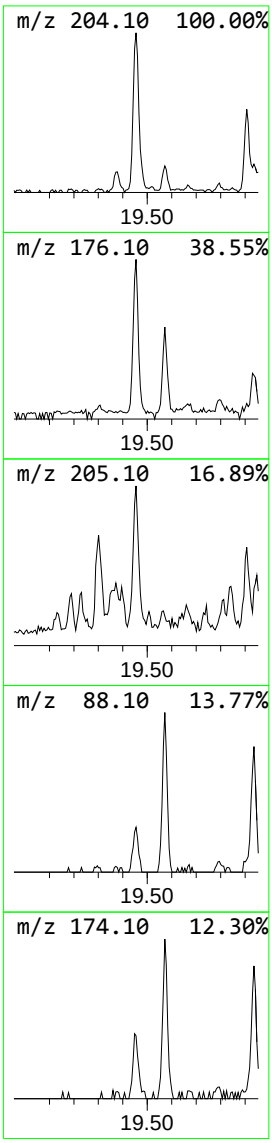
****

Peak Number 4 Cyclopenta(def)phenanthrenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.454	2.37 ng	69056	Phenanthrene-d10	17.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	95
2	5,6,7,8-Tetrahydrothieno[2,3-b]q...	204	C11H12N2S	122914-50-5	64
3	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	58
4	(E)-Ethyl 3-oxo-2-(pyrid-2-yl)me...	219	C12H13NO3	1000147-59-7	45
5	1,2-Dihydro-4-methyl-6-nitro-2-o...	204	C10H8N2O3	090771-17-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

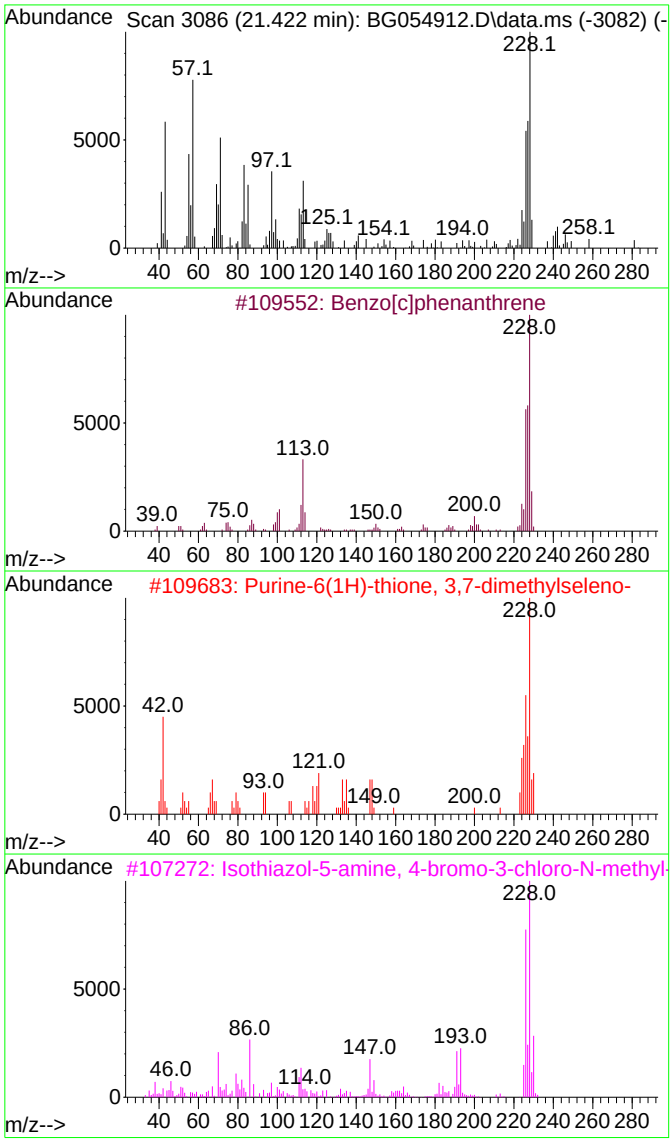
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

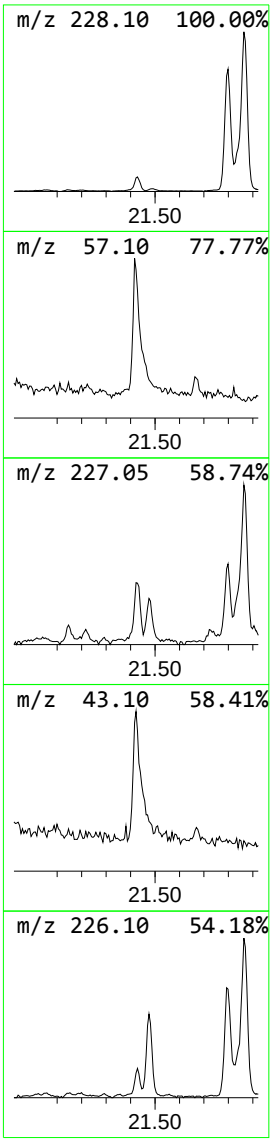
****

Peak Number 5 unknown21.422 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.422	2.05 ng	95896	Chrysene-d12	21.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]phenanthrene	228	C18H12	000195-19-7	38
2	Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	35
3	Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	30
4	Carbonic acid, 2-ethylhexyl hexa...	398	C25H50O3	1000383-14-3	27
5	L-Norvaline, N-(2-ethylhexyloxyc...	329	C18H35NO4	1000393-03-1	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

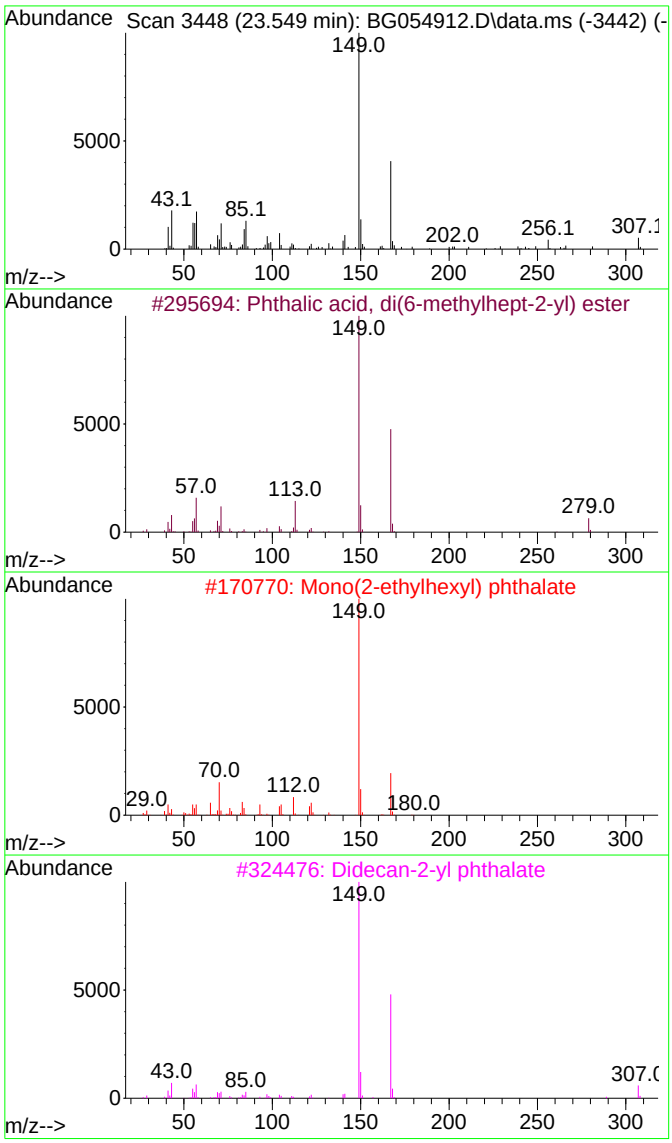
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

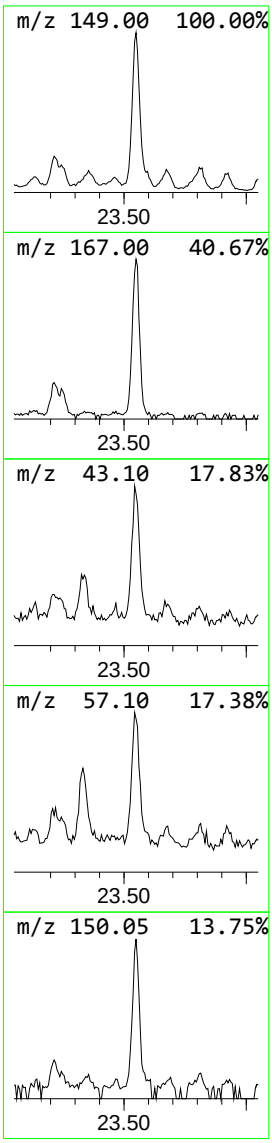
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phthalic acid, di(6-methylh... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.549	4.17 ng	154966	Perylene-d12	25.194

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, di(6-methylhept-2...	390	C24H38O4	1000377-97-3	72
2	Mono(2-ethylhexyl) phthalate	278	C16H22O4	004376-20-9	64
3	Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	64
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	64
5	Phthalic acid, di(2-propylpentyl...	390	C24H38O4	1000377-93-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

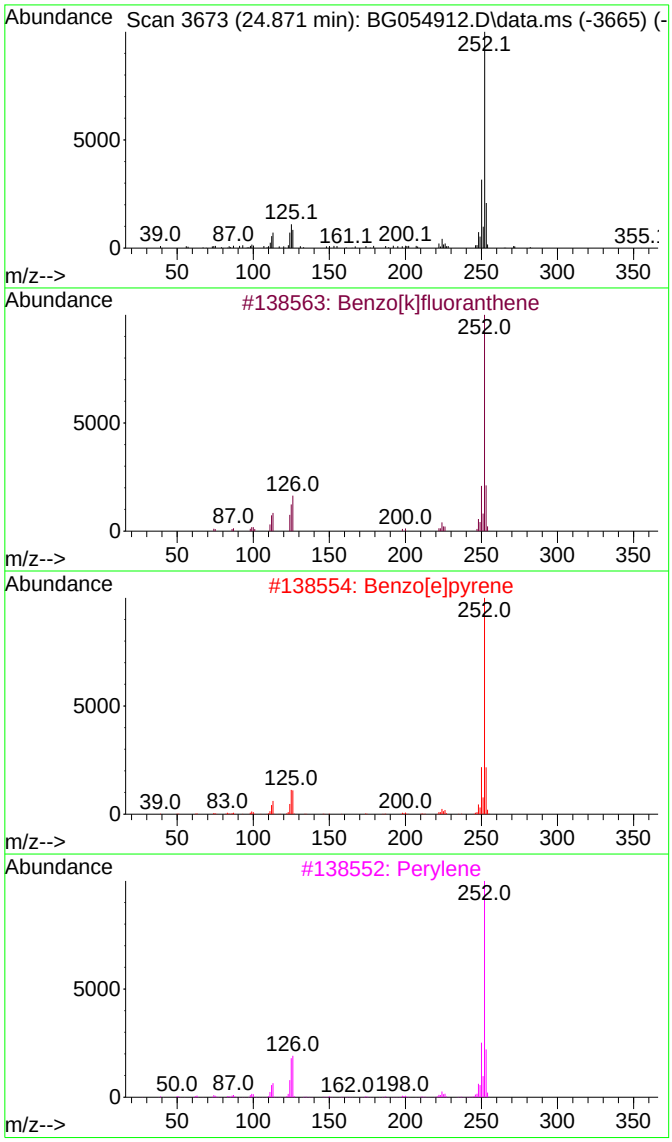
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

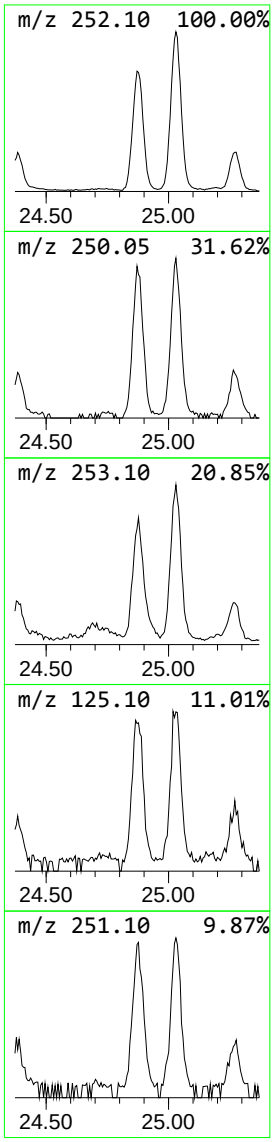
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.871	4.87 ng	181162	Perylene-d12	25.194

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2	Benzo[e]pyrene	252	C20H12	000192-97-2	96
3	Perylene	252	C20H12	000198-55-0	94
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
Data File : BG054912.D
Acq On : 12 Sep 2022 18:55
Operator : CG/JU
Sample : N4572-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PSC-124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
2-Pentanone, 4-...	5.200	9.7	ng	92485	1	8.138	191652	20.0
Ethanol, 2-(2-b...	10.717	5.8	ng	83610	2	10.970	285903	20.0
4H-Cyclopenta[d...	18.596	2.2	ng	65233	4	17.527	583286	20.0
Cyclopenta(def)...	19.454	2.4	ng	69056	4	17.527	583286	20.0
unknown21.422	21.422	2.0	ng	95896	5	21.816	936273	20.0
Phthalic acid, ...	23.549	4.2	ng	154966	6	25.194	743397	20.0
Benzo[e]pyrene	24.871	4.9	ng	181162	6	25.194	743397	20.0