LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139128.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	16	26	34	rVB	705793	1156500	57.26%	6.756%
2	5.128	506	516	525	rVB	82577	133373	6.60%	0.779%
3	5.522	576	583	588	rBV	1529215	2019835	100.00%	11.799%
4	6.522	746	753	763	rVB	1460196	2016973	99.86%	11.782%
5	6.898	812	817	822	rVB	401117	477326	23.63%	2.788%
6	7.457	906	912	917	rBV	959488	1221375	60.47%	7.135%
7	8.181	1029	1035	1040	rBV	455315	561311	27.79%	3.279%
8	8.486	1083	1087	1096	rVB	26008	32647	1.62%	0.191%
9	9.251	1212	1217	1222	rBV	1354841	1747612	86.52%	10.209%
10	9.933	1328	1333	1337	rBV	432350	529746	26.23%	3.095%
11	10.027	1342	1349	1354	rBV	22632	34125	1.69%	0.199%
12	10.716	1461	1466	1472	rBV	773749	990702	49.05%	5.787%
13	11.416	1580	1585	1588	rBV	374134	537850	26.63%	3.142%
14	11.492	1594	1598	1601	rBV	22838	25906	1.28%	0.151%
15	11.945	1667	1675	1680	rBV2	70385	115969	5.74%	0.677%
16	12.033	1686	1690	1698	rVB2	43295	67138	3.32%	0.392%
17	12.233	1717	1724	1728	rVB2	23456	46009	2.28%	0.269%
18	12.633	1786	1792	1797	rBV	437860	574082	28.42%	3.354%
19	12.727	1805	1808	1814	rBV2	19459	32823	1.63%	0.192%
20	12.857	1822	1830	1836	rBV	346530	549754	27.22%	3.211%
21	12.904	1836	1838	1846	rVB2	24758	31410	1.56%	0.183%
22	13.004	1846	1855	1860	rBV	1140817	1443758	71.48%	8.434%
23	13.074	1860	1867	1871	rBV2	19281	37842	1.87%	0.221%
24	13.186	1879	1886	1890	rBV	54386	77845	3.85%	0.455%
25	13.251	1893	1897	1901	rBV	50962	71647	3.55%	0.419%
26	13.804	1986	1991	1994	rBV	49537	82638	4.09%	0.483%
27	13.904	2003	2008	2014	rVB5	57438	96871	4.80%	0.566%
28	13.968	2015	2019	2023	rBV2	49072	60805	3.01%	0.355%
29	14.010	2023	2026	2028	rBV	18761	24329	1.20%	0.142%
30	14.057	2028	2034	2045	rVB2	439608	918522	45.48%	5.366%
31	14.163	2048	2052	2055	rBV	31905	38056	1.88%	0.222%
32	14.539	2112	2116	2119	rBV4	26016	39055	1.93%	0.228%
33	14.592	2122	2125	2129	rVB2	41126	52451	2.60%	0.306%
34	15.104	2206	2212	2223	rVV	143168	333532	16.51%	1.948%
35	15.198	2224	2228	2236	rVB3	44573	86691	4.29%	0.506%
36	15.409	2259	2264	2269	rVB	69476	105948	5.25%	0.619%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

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-BF082024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.468	2269	2274	2279	rVV	91981	137166	6.79%	0.801%
38	15.533	2280	2285	2298	rVB	217220	389220	19.27%	2.274%
39	16.033	2367	2370	2375	rVB	22054	33241	1.65%	0.194%
40	17.009	2532	2536	2546	rVB2	45520	101383	5.02%	0.592%
41	17.456	2607	2612	2629	rVB	33562	84913	4.20%	0.496%

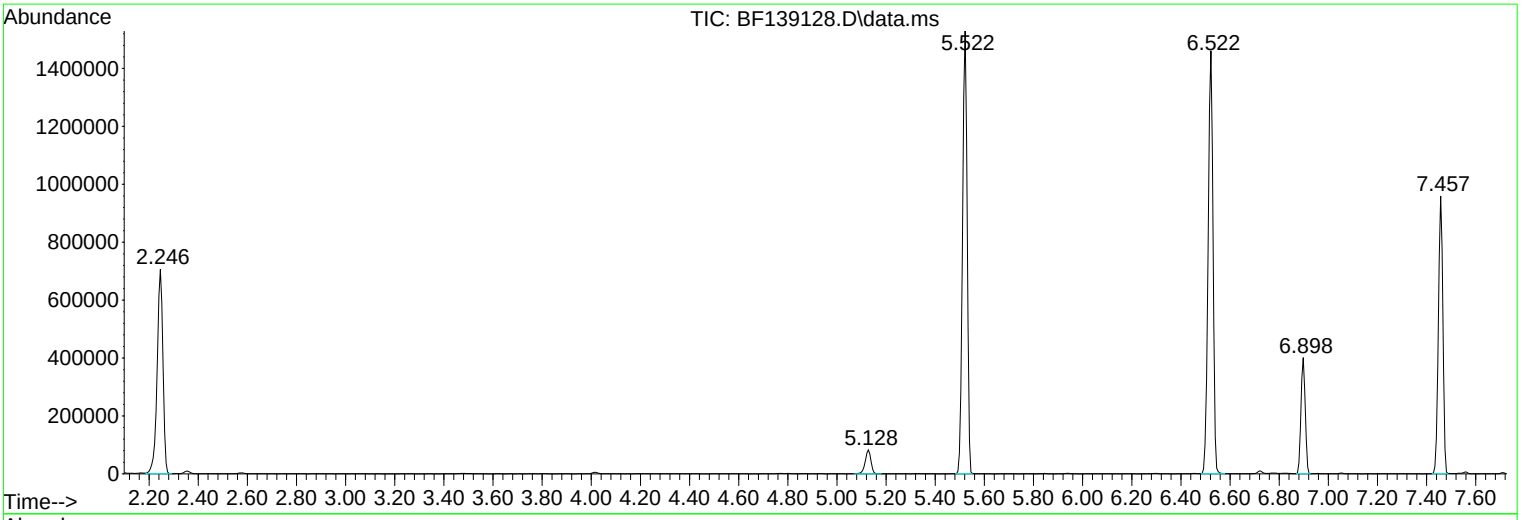
Sum of corrected areas: 17118379

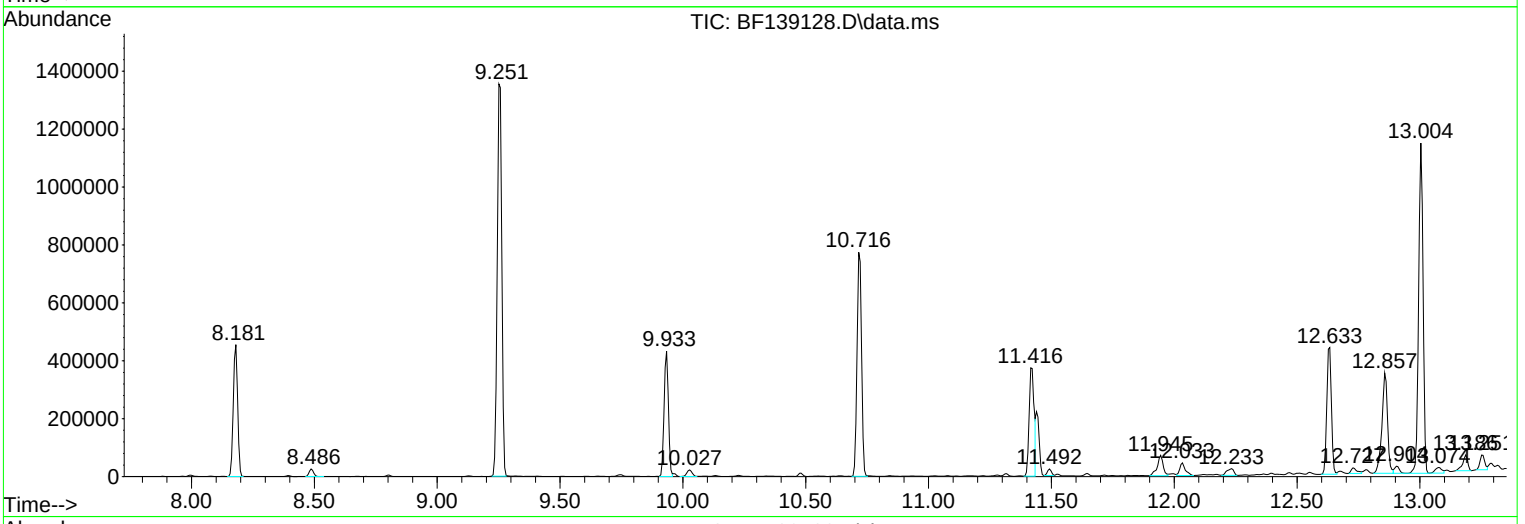
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

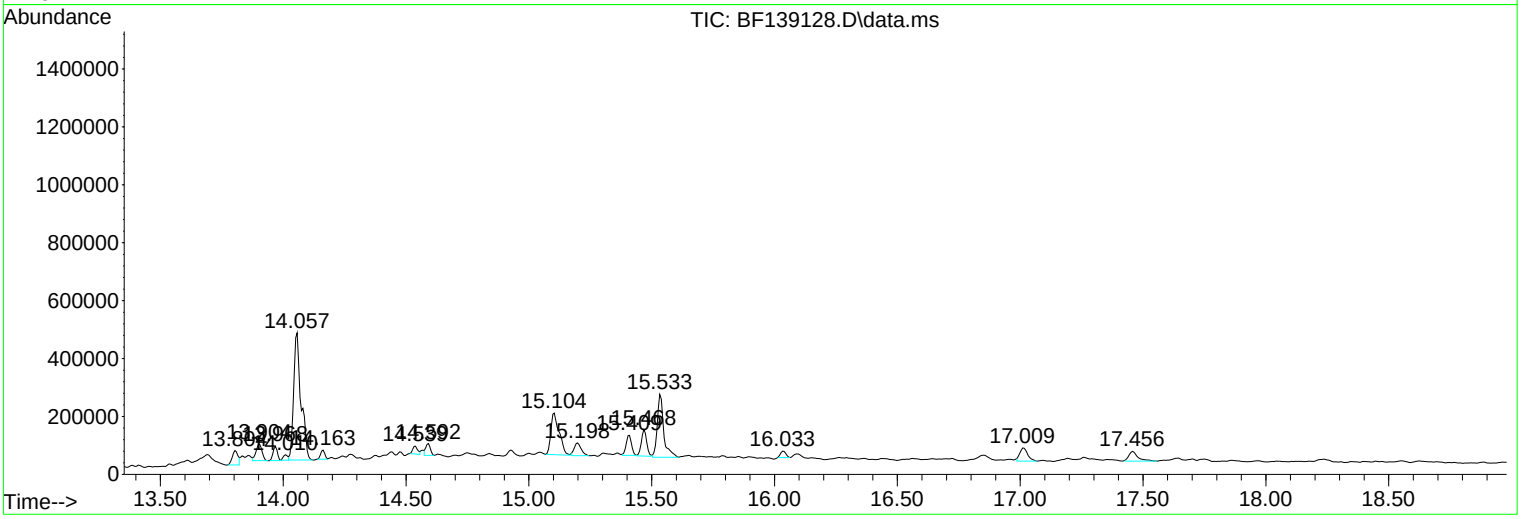
Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

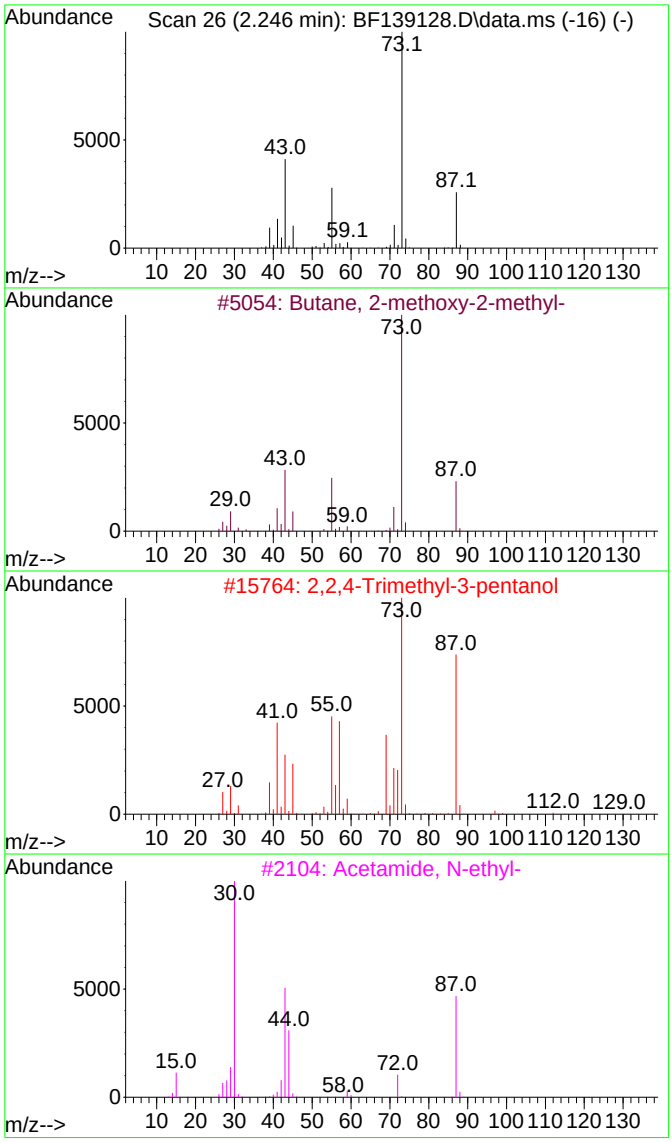
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

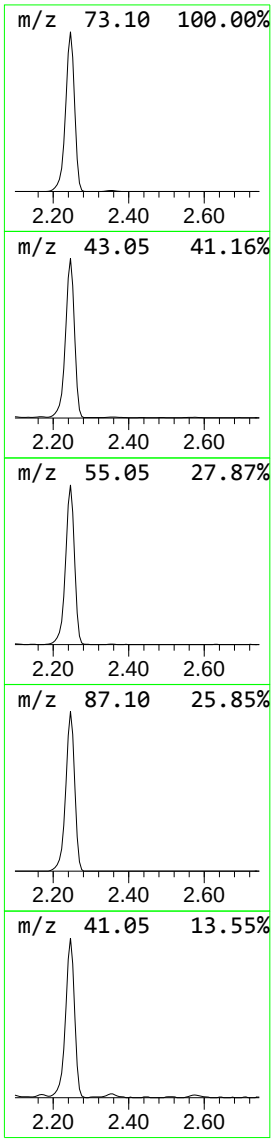
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	48.46 ng	1156500	1,4-Dichlorobenzene-d4	6.898

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

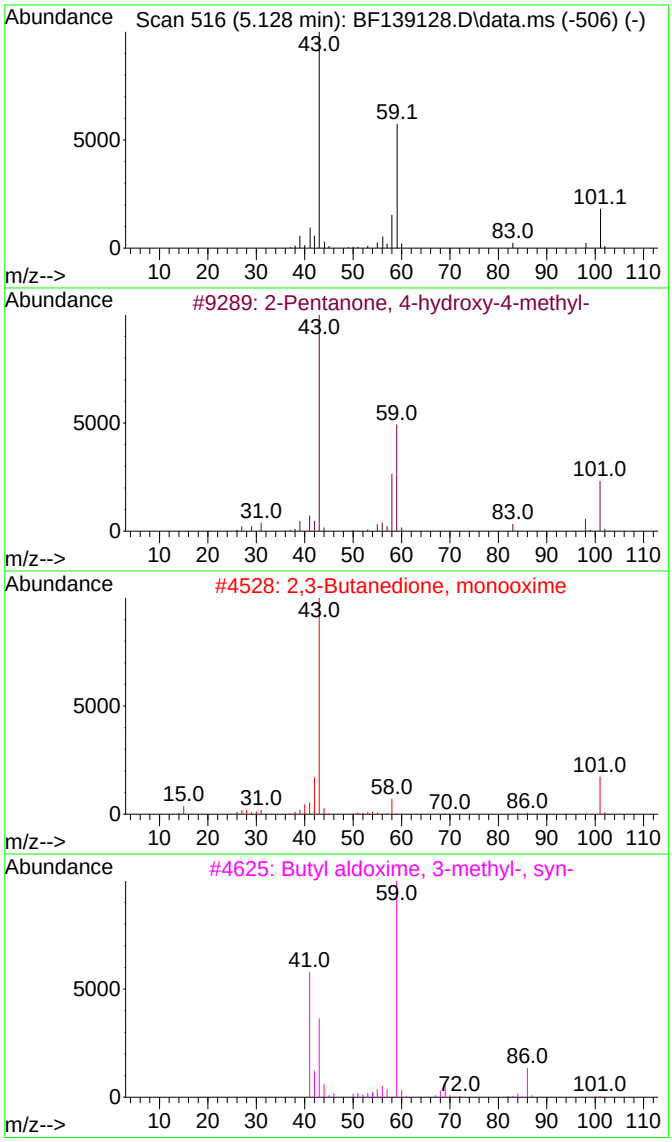
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

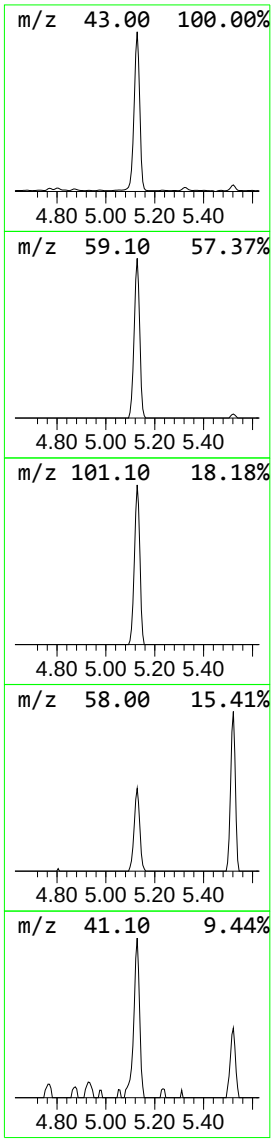
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	5.59 ng	133373	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Acetamide, N-(cyanomethyl)-	98	C4H6N2O	004814-80-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

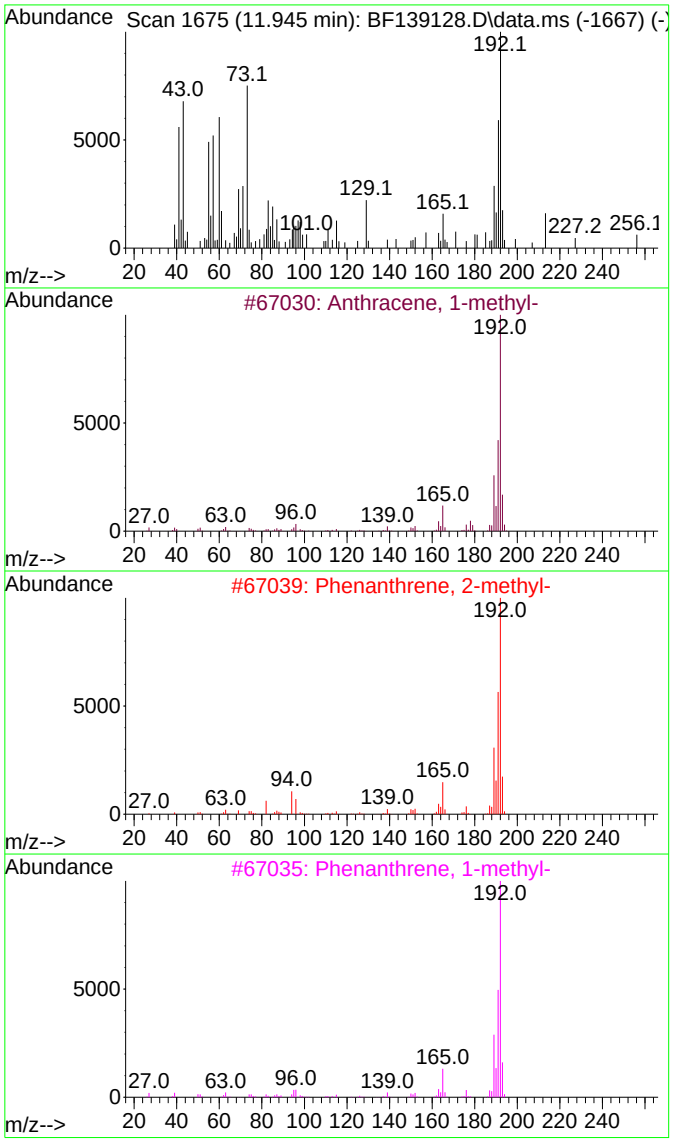
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

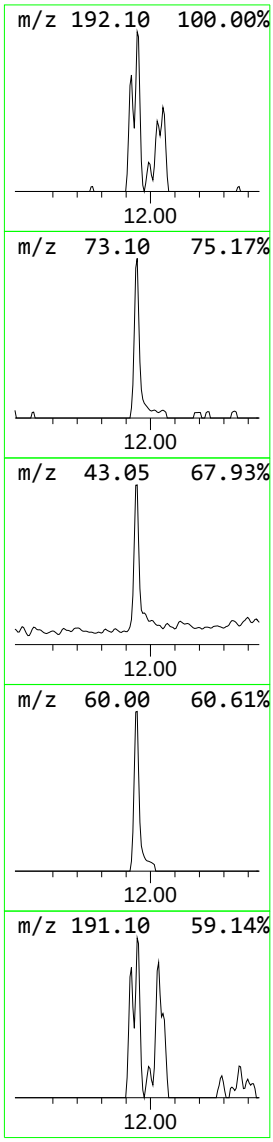
****

Peak Number 3 Anthracene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	4.31 ng	115969	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	89
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	89
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

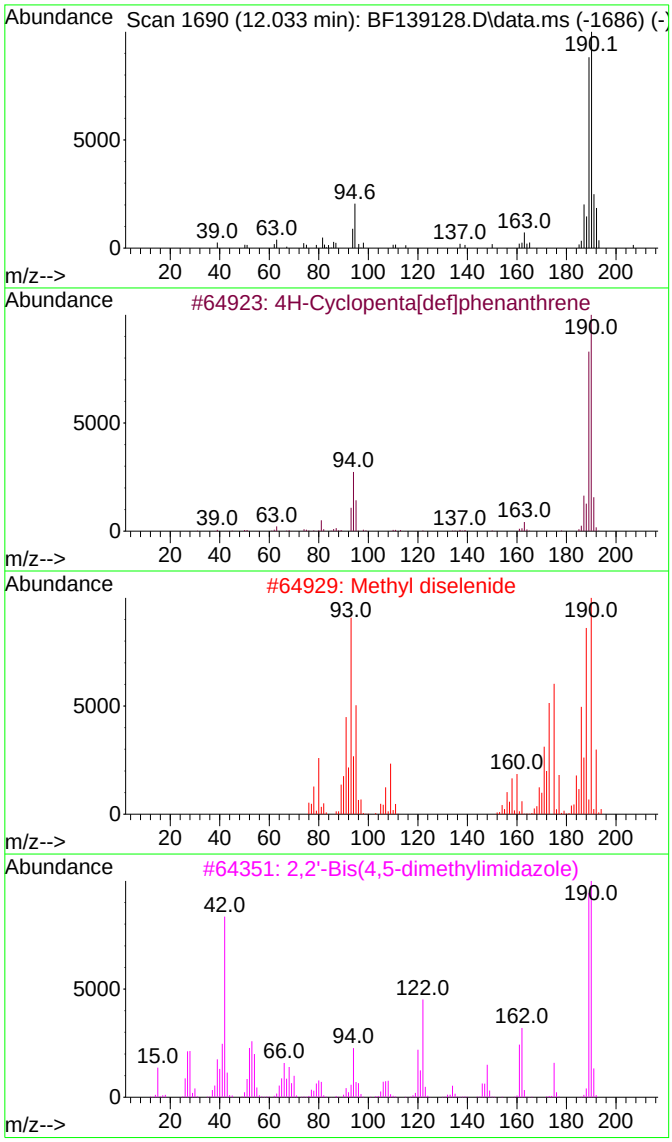
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

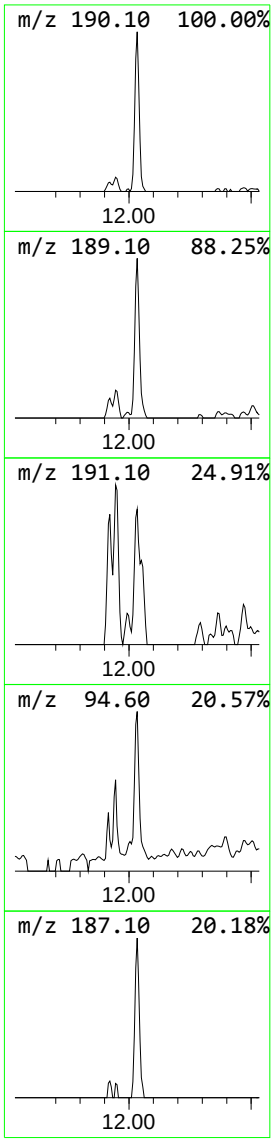
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.50 ng	67138	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	94
2	Methyl diselenide	190	C2H6Se2	007101-31-7	49
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4	Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	40
5	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	37





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

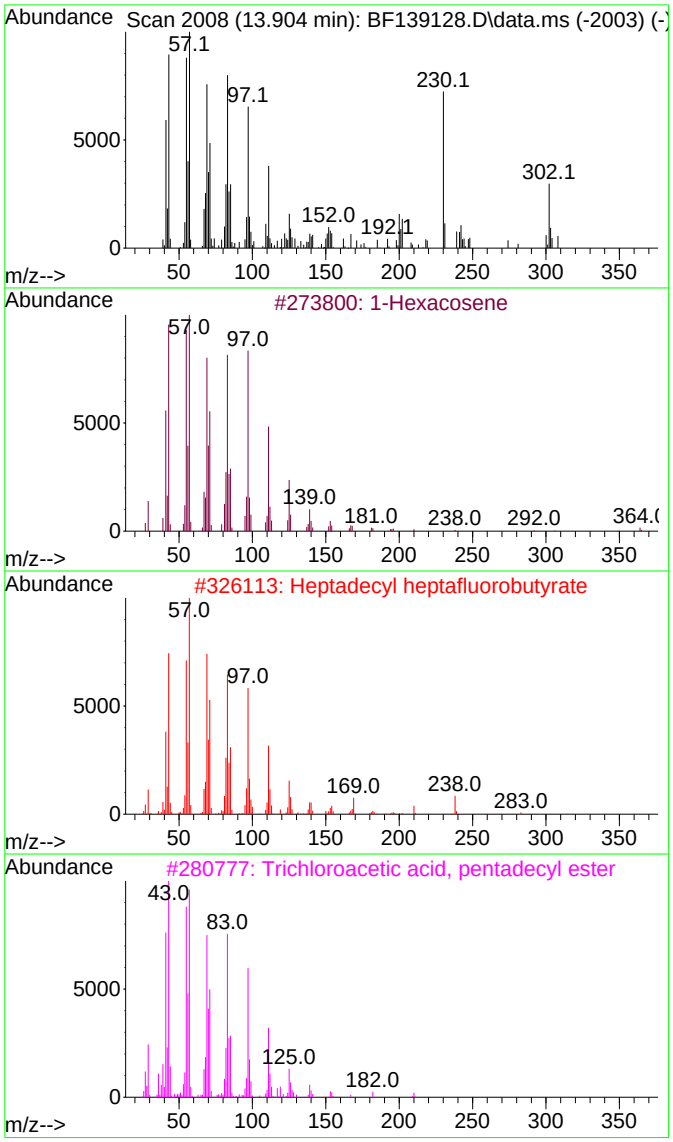
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

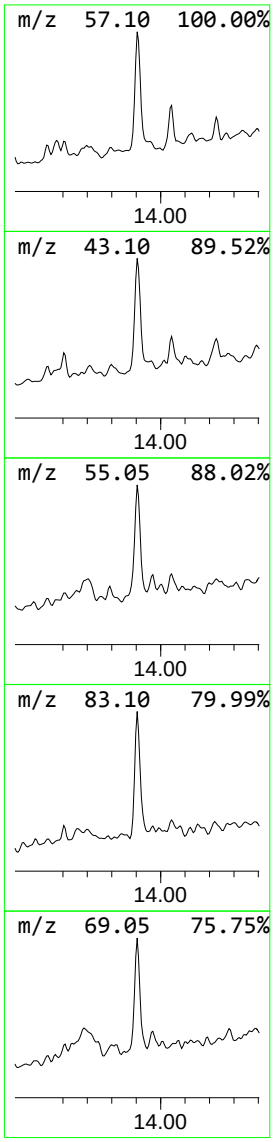
****

Peak Number 5 1-Hexacosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.11 ng	96871	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	90
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

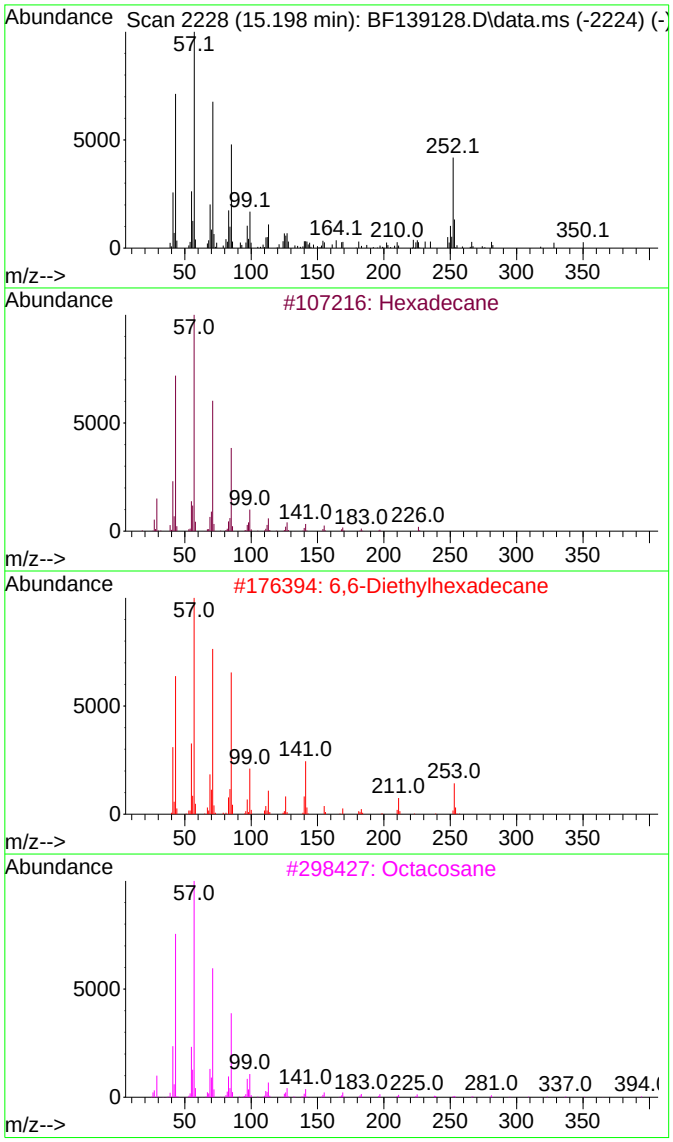
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

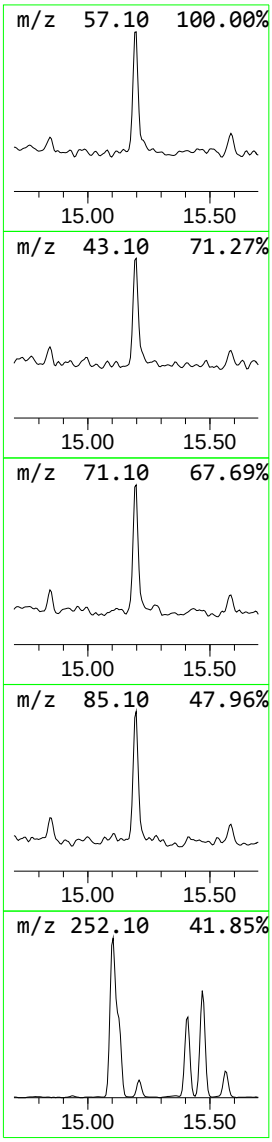
****

Peak Number 6 Hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	4.45 ng	86691	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	6,6-Diethylhexadecane	282	C20H42	1000360-41-4	52
3	Octacosane	394	C28H58	000630-02-4	49
4	Tetracosane	338	C24H50	000646-31-1	49
5	Hentriacontane	437	C31H64	000630-04-6	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

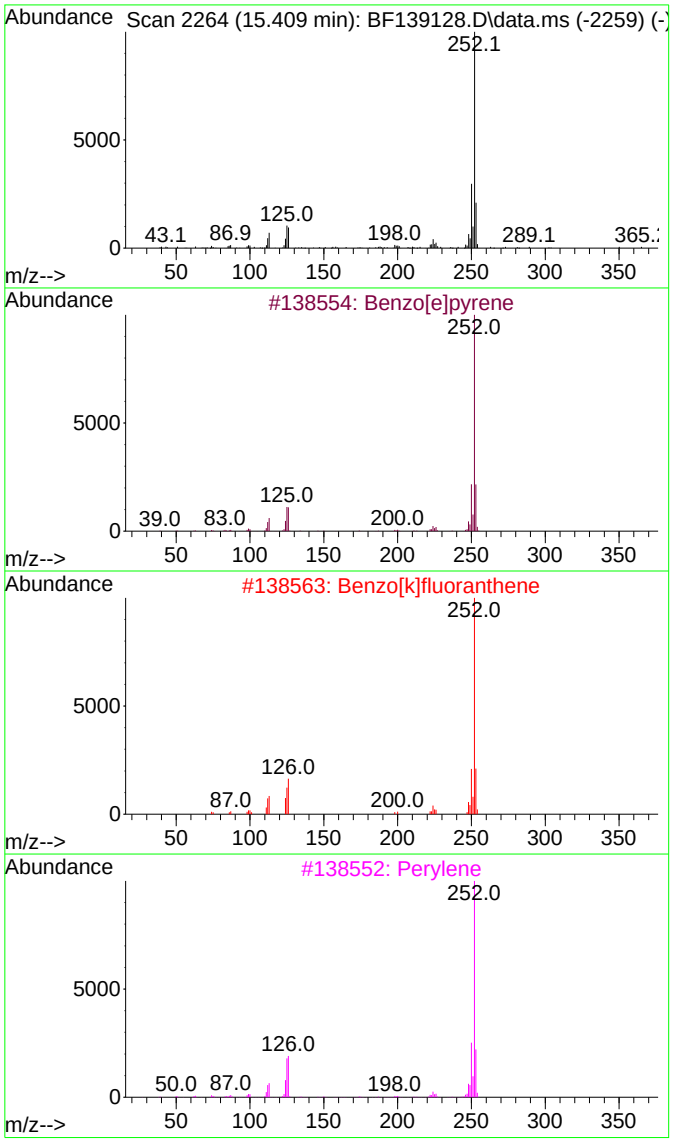
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

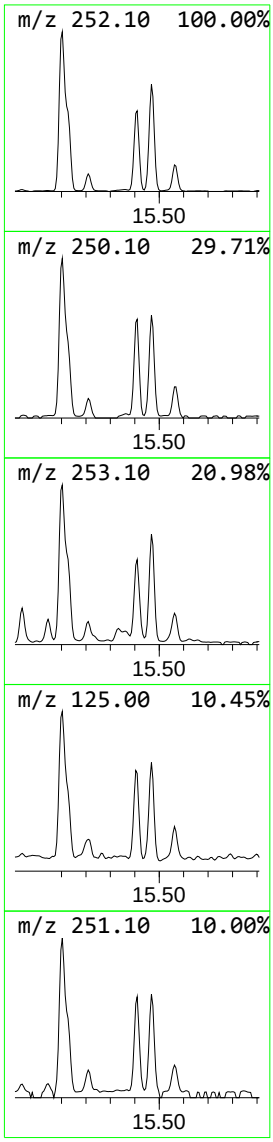
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	5.44 ng	105948	Perylene-d12	15.533

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Perylene	252	C20H12	000198-55-0	94
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082224\
Data File : BF139128.D
Acq On : 22 Aug 2024 17:51
Operator : RC/JU
Sample : P3663-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
919-J-SD-0-1-081624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082024.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...	2.246	48.5	ng	1156500	1	6.898	477326	20.0
2-Pentanone, 4-...	5.128	5.6	ng	133373	1	6.898	477326	20.0
Anthracene, 1-m...	11.945	4.3	ng	115969	4	11.416	537850	20.0
4H-Cyclopenta[d...	12.033	2.5	ng	67138	4	11.416	537850	20.0
1-Hexacosene	13.904	2.1	ng	96871	5	14.057	918522	20.0
Hexadecane	15.198	4.5	ng	86691	6	15.533	389220	20.0
Benzo[e]pyrene	15.410	5.4	ng	105948	6	15.533	389220	20.0