

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
 Data File : BP020502.D
 Acq On : 04 Jun 2024 18:57
 Operator : MA/JU
 Sample : P2680-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RBR2520258

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_P\Methods\8270E-BP052924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020502.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	4	9	27	rVB	2037413	2777954	30.61%	3.498%
2	4.928	324	330	338	rVB	124990	178472	1.97%	0.225%
3	5.369	397	405	418	rBV	2684788	4050071	44.63%	5.101%
4	6.928	662	670	688	rBV	2736917	4397104	48.46%	5.538%
5	7.757	803	811	818	rBV	957000	1538039	16.95%	1.937%
6	8.904	998	1006	1016	rBV	1616939	2748515	30.29%	3.461%
7	10.528	1272	1282	1289	rBV	1345629	2162777	23.84%	2.724%
8	12.993	1694	1701	1709	rBV	4094949	6051043	66.69%	7.621%
9	14.387	1930	1938	1945	rBV	1863515	2872108	31.65%	3.617%
10	15.892	2188	2194	2207	rBV	2786285	4086845	45.04%	5.147%
11	17.192	2409	2415	2419	rBV	2358236	3457634	38.11%	4.354%
12	17.233	2419	2422	2428	rVB	340470	495926	5.47%	0.625%
13	17.328	2434	2438	2446	rBV	126325	209040	2.30%	0.263%
14	18.139	2572	2576	2585	rBV	270320	379252	4.18%	0.478%
15	19.322	2772	2777	2785	rVB	1155471	1670864	18.41%	2.104%
16	19.475	2800	2803	2808	rVB5	95835	133014	1.47%	0.168%
17	19.698	2832	2841	2851	rBV	1276845	2028759	22.36%	2.555%
18	19.933	2875	2881	2890	rVB	6174468	9073856	100.00%	11.427%
19	20.045	2897	2900	2907	rVB2	141845	263850	2.91%	0.332%
20	20.216	2919	2929	2937	rVB3	288638	835192	9.20%	1.052%
21	20.322	2944	2947	2951	rVB2	168721	201951	2.23%	0.254%
22	20.380	2953	2957	2963	rVB2	237435	369834	4.08%	0.466%
23	20.527	2979	2982	2986	rVB	234881	275146	3.03%	0.347%
24	20.574	2987	2990	2995	rVB2	93999	146504	1.61%	0.185%
25	21.004	3060	3063	3073	rVB	203824	353913	3.90%	0.446%
26	21.204	3094	3097	3101	rVB	208833	308414	3.40%	0.388%
27	21.251	3101	3105	3108	rVV	212266	265063	2.92%	0.334%
28	21.292	3109	3112	3116	rVV2	153883	287641	3.17%	0.362%
29	21.333	3116	3119	3134	rVB3	307026	715690	7.89%	0.901%
30	21.580	3158	3161	3163	rBV2	115875	156651	1.73%	0.197%
31	21.639	3163	3171	3176	rVV2	2512759	6483532	71.45%	8.165%
32	21.692	3176	3180	3191	rVB	1290177	2444392	26.94%	3.078%
33	22.410	3299	3302	3308	rVB	252522	428919	4.73%	0.540%
34	22.492	3311	3316	3322	rVB2	230845	433517	4.78%	0.546%
35	22.963	3390	3396	3410	rBV	444579	1169310	12.89%	1.473%
36	23.927	3552	3560	3569	rBV	1549357	4888884	53.88%	6.157%

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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_P\Methods\8270E-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	24.204	3603	3607	3613	rVB2	122281	207570	2.29%	0.261%
38	24.680	3680	3688	3698	rVB	949179	2384040	26.27%	3.002%
39	24.833	3706	3714	3726	rVB	850909	2139049	23.57%	2.694%
40	24.998	3731	3742	3750	rBV	1491568	4172346	45.98%	5.255%
41	28.786	4377	4386	4387	rBV	305900	647919	7.14%	0.816%
42	29.939	4573	4582	4601	rVB	332993	1513982	16.69%	1.907%

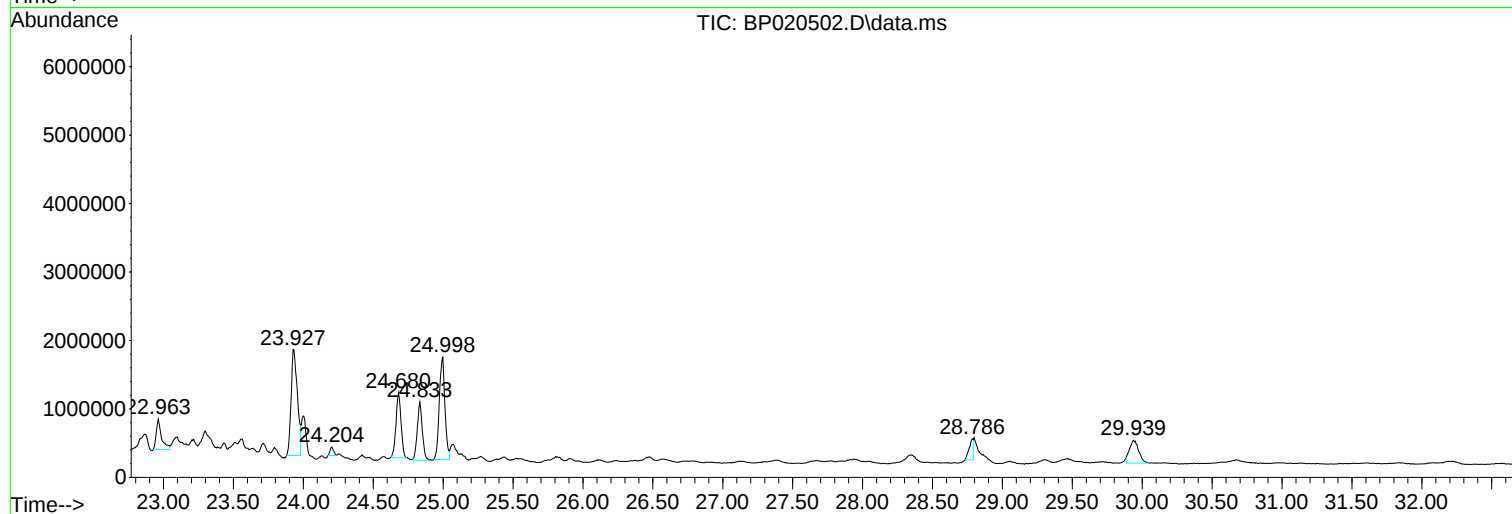
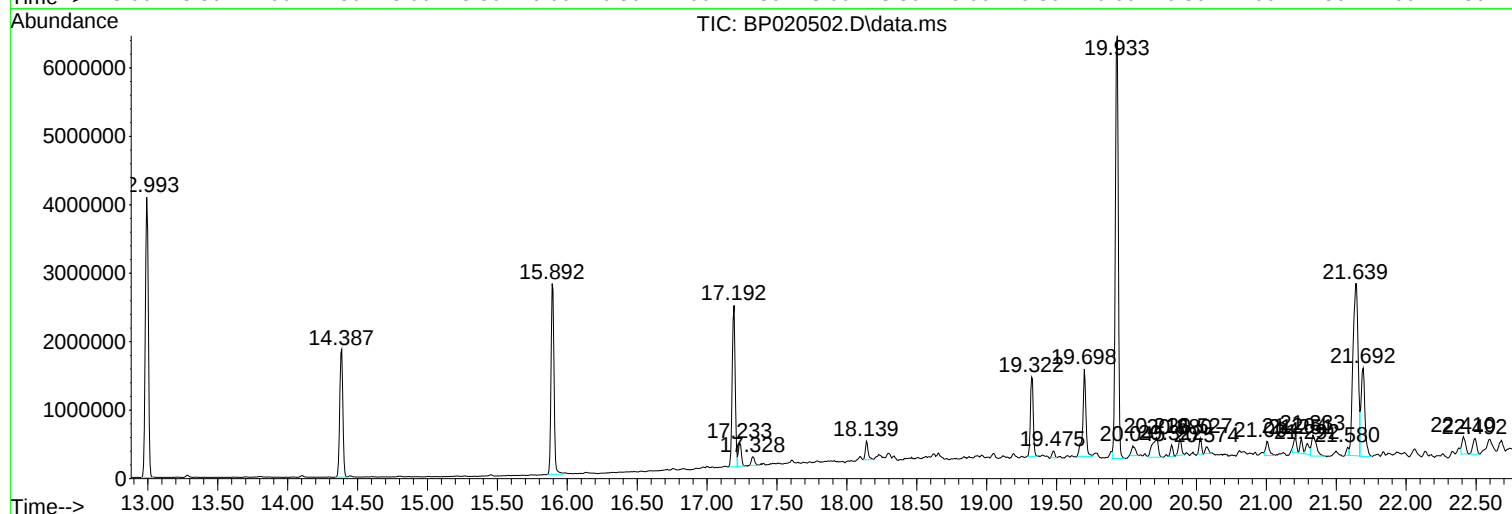
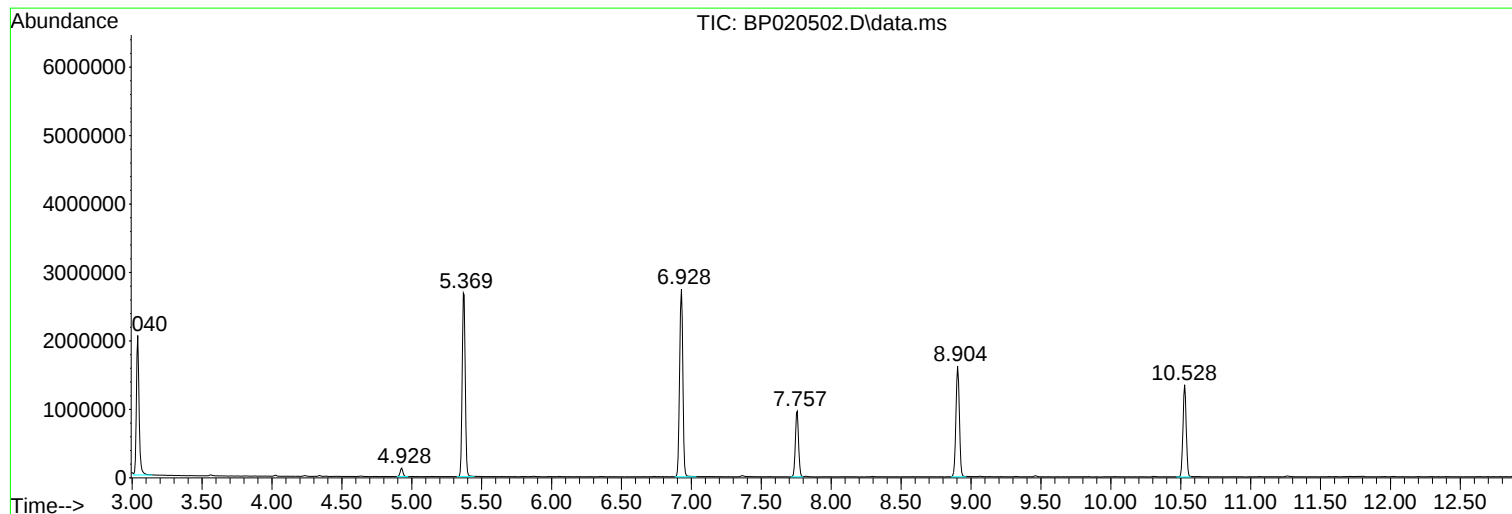
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : MA/JU
Sample : P2680-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR2520258

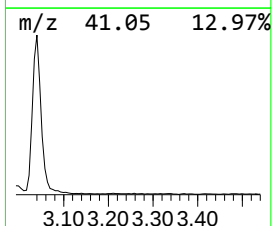
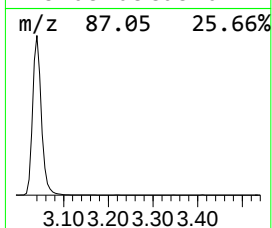
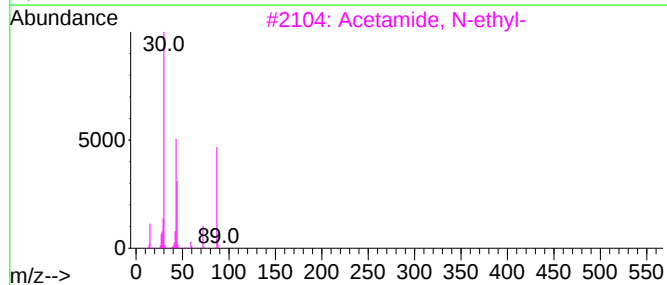
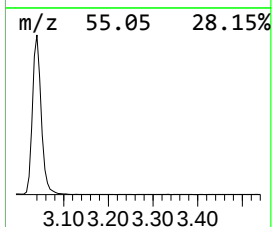
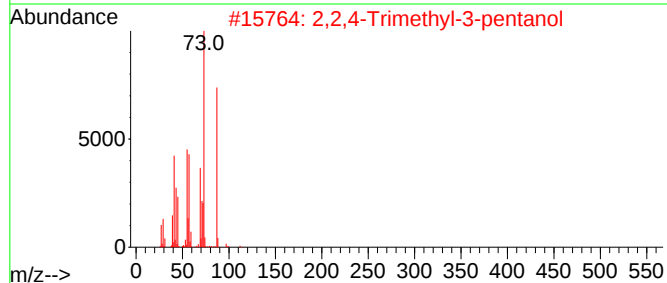
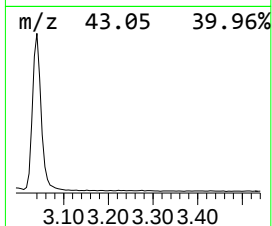
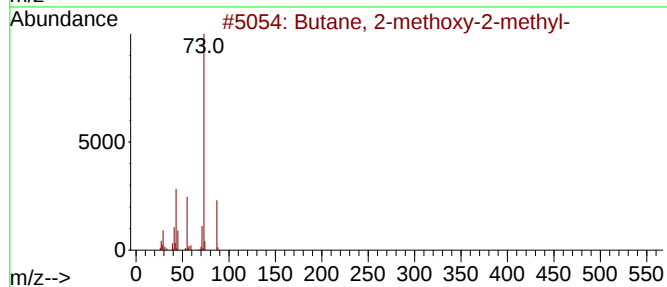
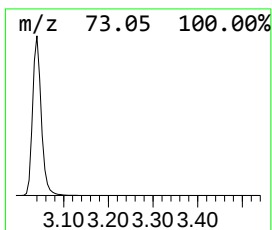
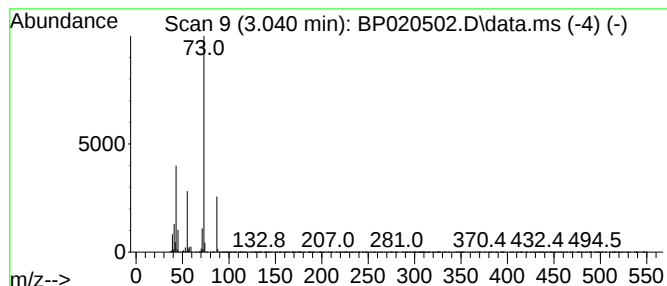
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.040	36.12 ng	2777950	1,4-Dichlorobenzene-d4	7.757

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



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR2520258

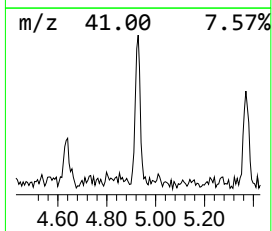
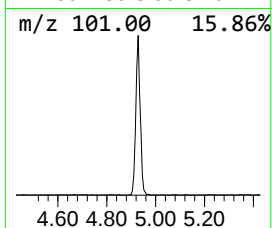
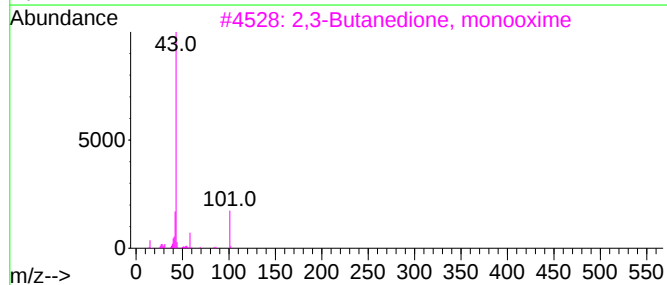
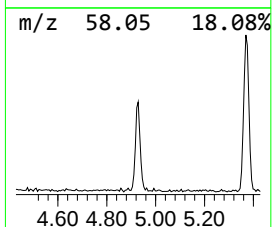
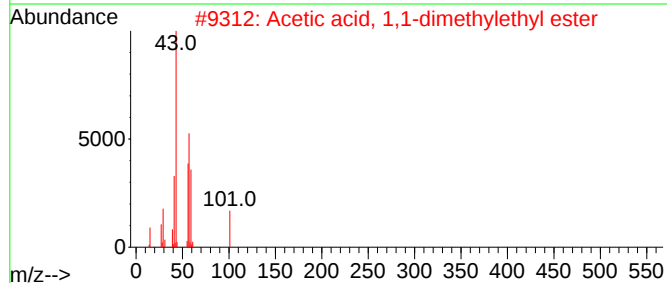
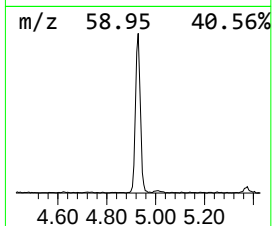
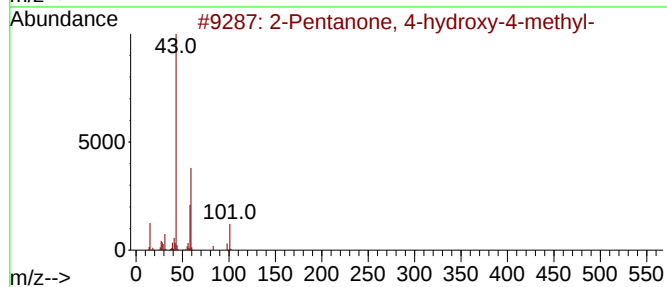
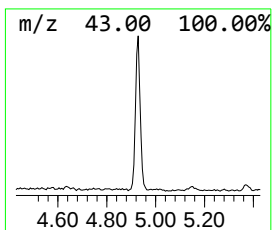
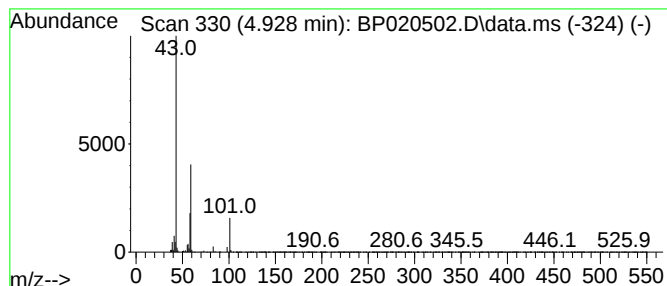
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.928	2.32 ng	178472	1,4-Dichlorobenzene-d4	7.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	74
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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Instrument :
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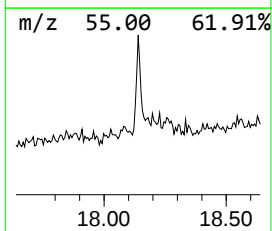
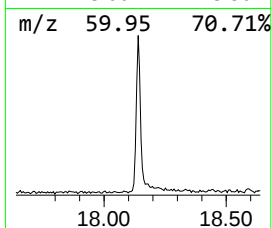
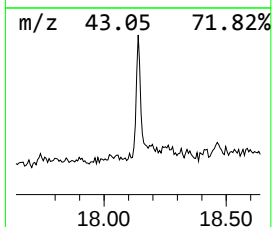
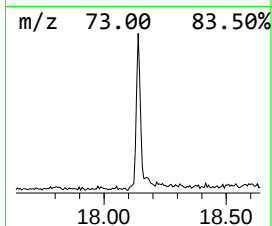
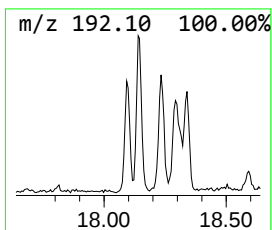
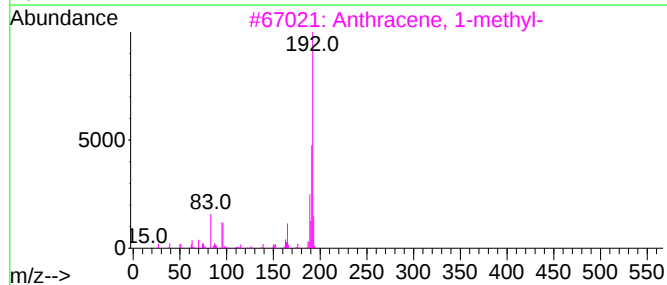
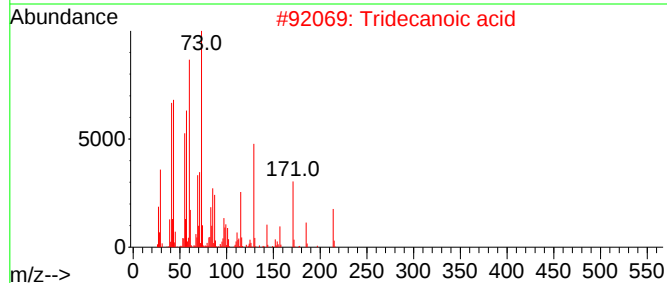
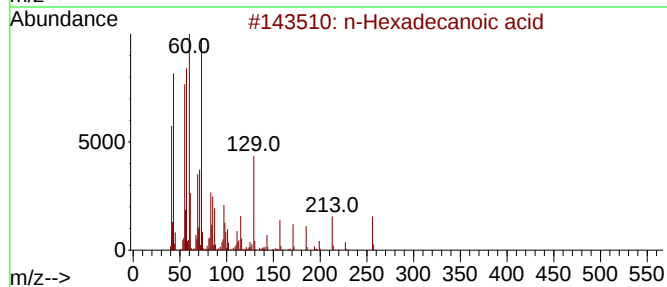
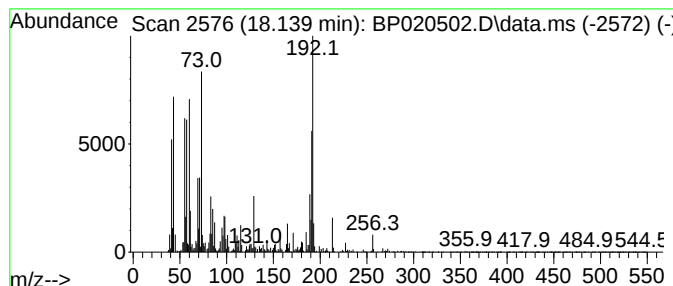
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	2.19 ng	379252	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	83
3			Anthracene, 1-methyl-	192	C15H12	000610-48-0	62
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	62
5			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	60



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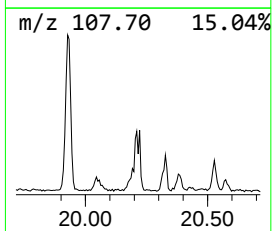
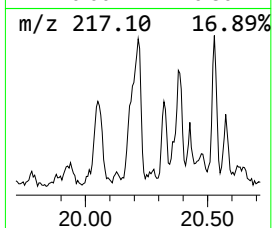
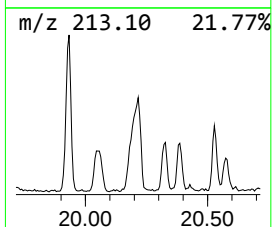
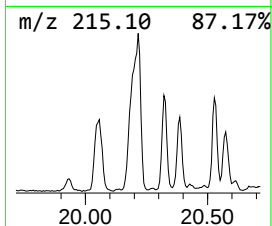
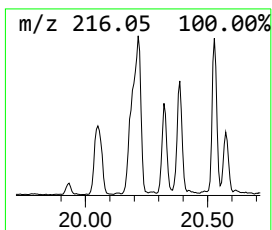
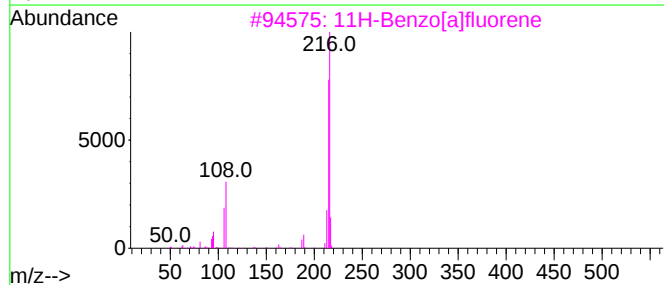
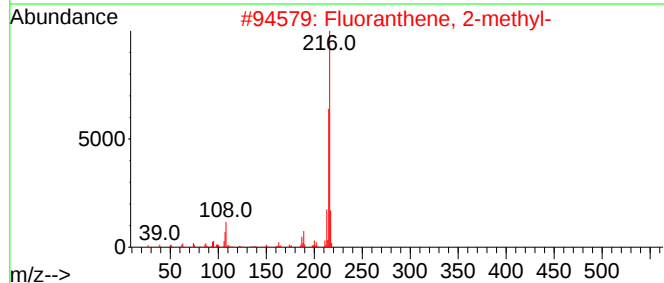
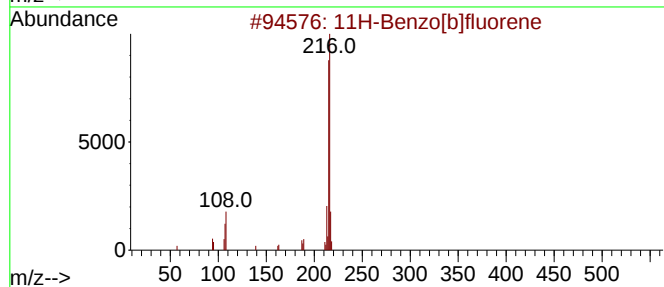
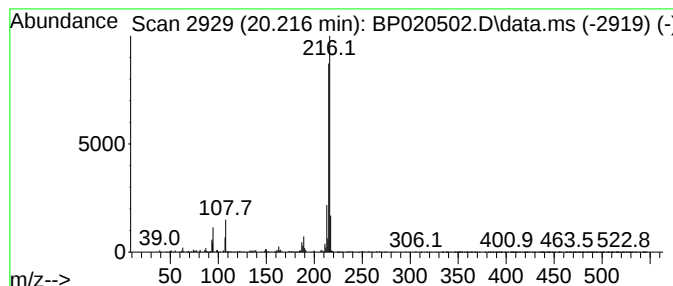
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.216	2.58 ng	835192	Chrysene-d12	21.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
2			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
3			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
4			Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72



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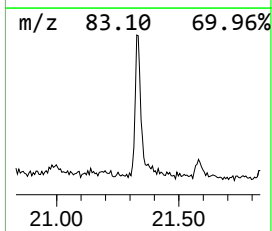
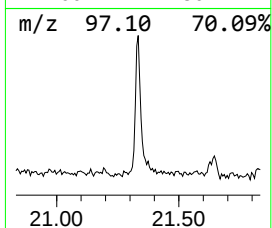
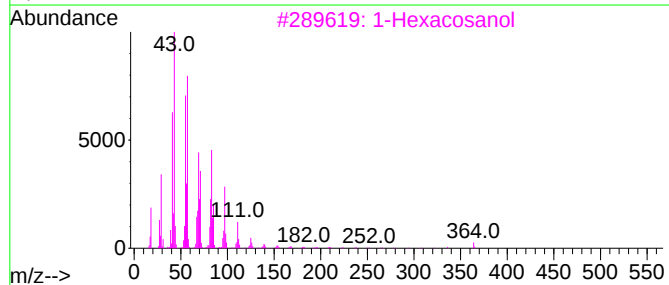
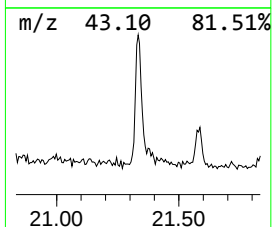
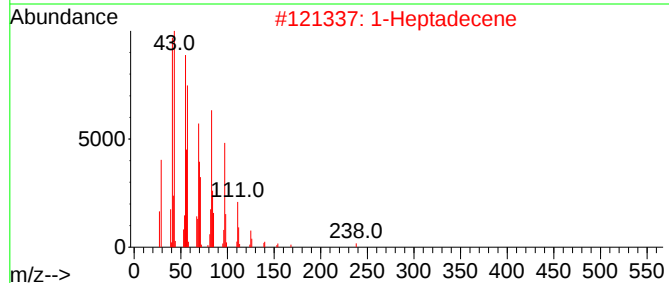
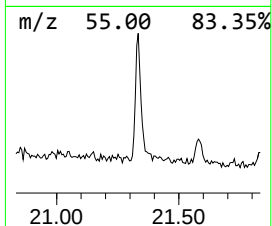
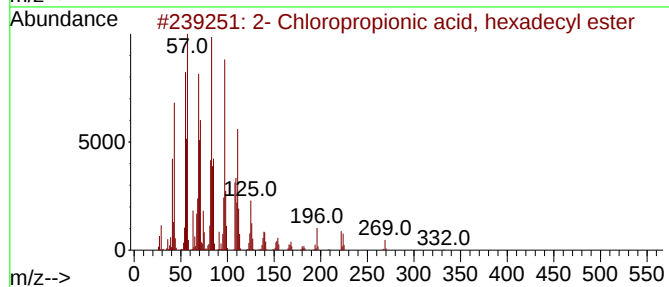
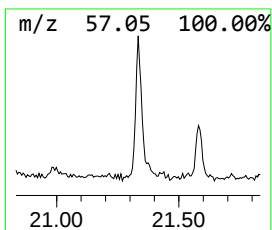
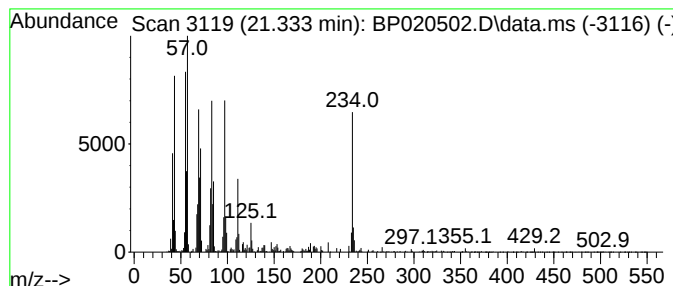
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2- Chloropropionic acid, he... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.333	2.21 ng	715690	Chrysene-d12	21.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	89
2			1-Heptadecene	238	C17H34	006765-39-5	78
3			1-Hexacosanol	382	C26H54O	000506-52-5	76
4			1-Heptacosanol	396	C27H56O	002004-39-9	76
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020502.D
Acq On : 04 Jun 2024 18:57
Operator : MA/JU
Sample : P2680-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

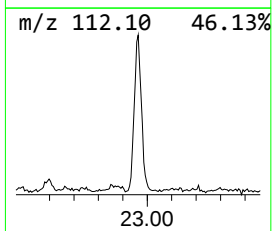
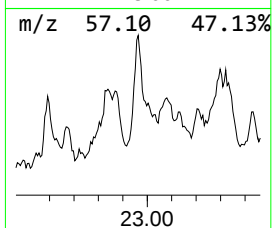
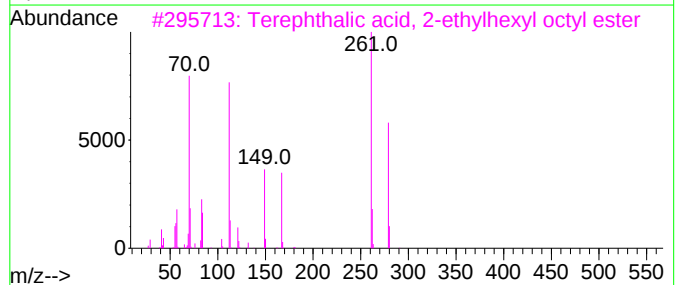
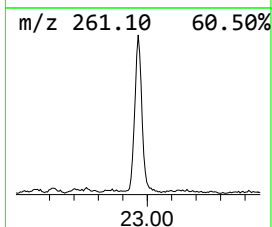
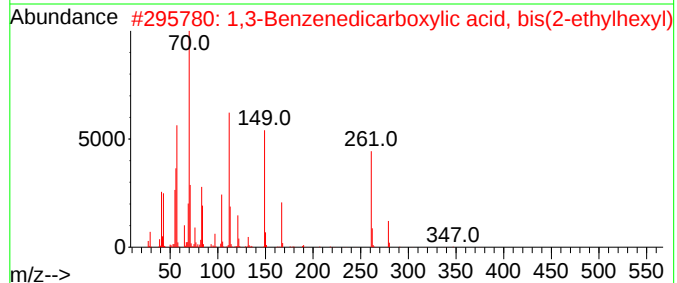
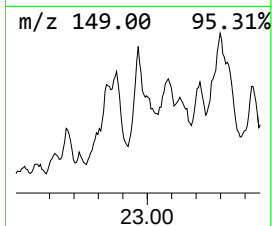
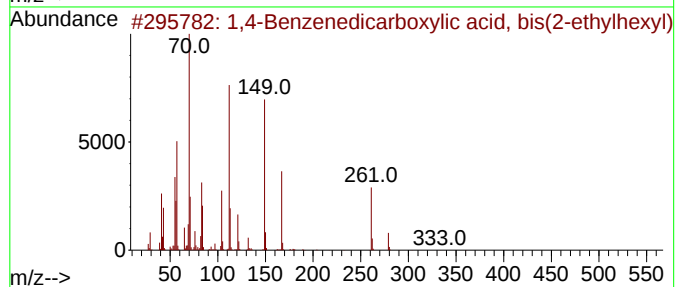
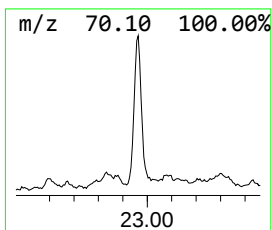
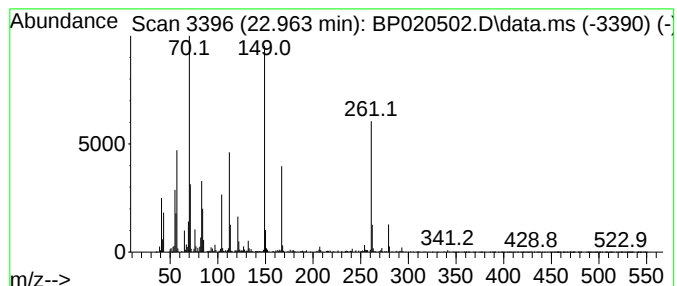
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ClientSampleId :
RBR2520258

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.963	3.61 ng	1169310	Chrysene-d12	21.645	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	81
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	62
3	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	58
4	Terephthalic acid, 4-cyanophenyl...	379	C23H25NO4	1000323-66-6	35
5	Phthalic acid, 3,4-dichloropheny...	422	C22H24Cl2O4	1000315-27-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020502.D
Acq On : 04 Jun 2024 18:57
Operator : MA/JU
Sample : P2680-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR2520258

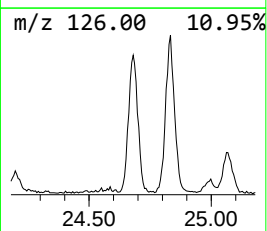
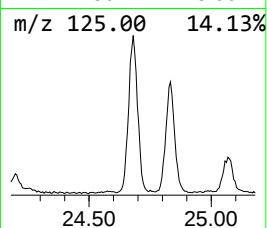
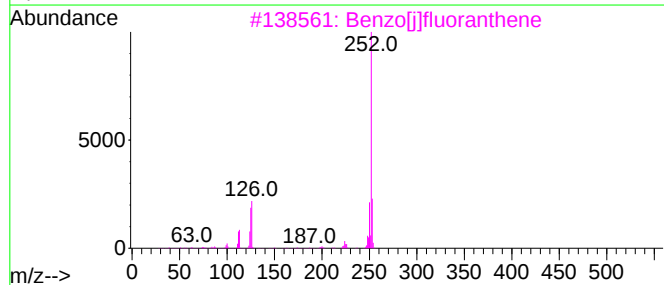
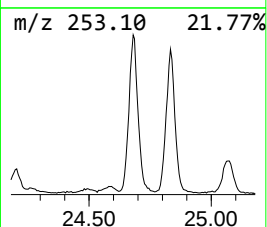
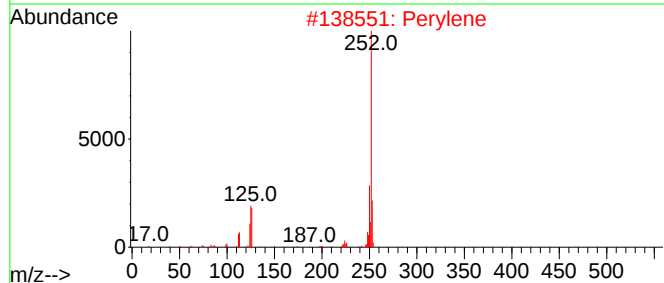
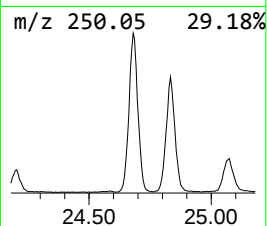
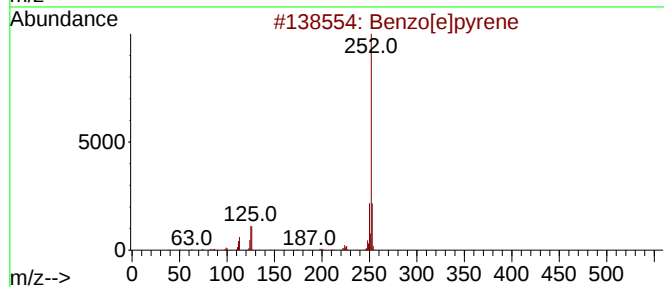
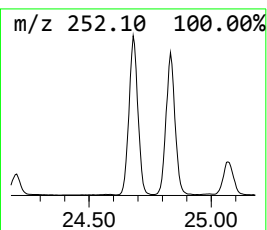
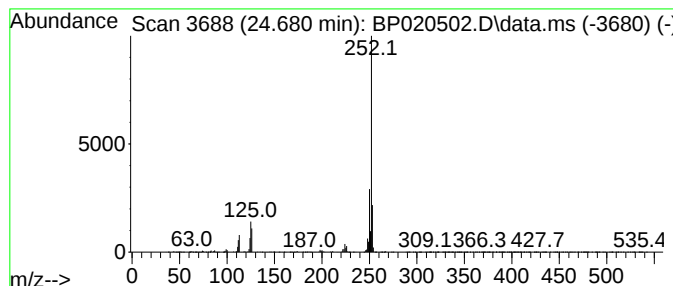
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.680	11.43 ng	2384040	Perylene-d12	24.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Perylene	252	C20H12	000198-55-0	95
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020502.D
Acq On : 04 Jun 2024 18:57
Operator : MA/JU
Sample : P2680-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RBR2520258

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.040	36.1	ng	2777950	1	7.757	1538040	20.0
2-Pentanone, 4-...	4.928	2.3	ng	178472	1	7.757	1538040	20.0
n-Hexadecanoic ...	18.139	2.2	ng	379252	4	17.192	3457630	20.0
11H-Benzo[b]flu...	20.216	2.6	ng	835192	5	21.645	6483530	20.0
2- Chloropropio...	21.333	2.2	ng	715690	5	21.645	6483530	20.0
1,4-Benzenedica...	22.963	3.6	ng	1169310	5	21.645	6483530	20.0
Benzo[e]pyrene	24.680	11.4	ng	2384040	6	24.998	4172350	20.0