

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
 Data File : BF125867.D
 Acq On : 15 Oct 2021 17:32
 Operator : JU/CG
 Sample : M4243-10
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T3-COMP-(1-4)

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-BF100721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125867.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	501	505	511	rVB	53514	69030	1.84%	0.149%
2	5.451	567	572	575	rBV	3109379	3085019	82.09%	6.639%
3	6.463	738	744	747	rBV	3152387	3156859	84.00%	6.793%
4	6.834	803	807	810	rBV	1268682	956123	25.44%	2.057%
5	7.392	897	902	905	rBV	2307930	2063158	54.90%	4.440%
6	8.016	1004	1008	1017	rBV	236760	225595	6.00%	0.485%
7	8.116	1021	1025	1027	rVV	1430449	1314679	34.98%	2.829%
8	8.134	1027	1028	1035	rVB	306013	190457	5.07%	0.410%
9	8.822	1142	1145	1149	rBV	190560	166468	4.43%	0.358%
10	8.922	1159	1162	1165	rBV	268009	201988	5.37%	0.435%
11	9.186	1203	1207	1210	rBV	4251086	3758269	100.00%	8.087%
12	9.286	1222	1224	1228	rBV2	61809	62513	1.66%	0.135%
13	9.381	1238	1240	1246	rBV2	79192	125289	3.33%	0.270%
14	9.457	1247	1253	1256	rVV5	99155	165741	4.41%	0.357%
15	9.522	1261	1264	1267	rVV	201628	219628	5.84%	0.473%
16	9.551	1267	1269	1274	rVB3	120527	135560	3.61%	0.292%
17	9.639	1282	1284	1286	rBV	86581	84614	2.25%	0.182%
18	9.728	1296	1299	1300	rBV2	111298	115223	3.07%	0.248%
19	9.804	1310	1312	1316	rBV4	73397	76140	2.03%	0.164%
20	9.863	1316	1322	1325	rBV	1453661	1558368	41.47%	3.353%
21	9.898	1325	1328	1331	rVB	778209	642716	17.10%	1.383%
22	9.928	1331	1333	1336	rBV3	98944	102697	2.73%	0.221%
23	10.069	1354	1357	1362	rBV	437242	394749	10.50%	0.849%
24	10.410	1412	1415	1418	rBV	523805	504823	13.43%	1.086%
25	10.651	1453	1456	1459	rBV	1804055	1759117	46.81%	3.785%
26	11.357	1573	1576	1577	rBV	910693	845840	22.51%	1.820%
27	11.380	1577	1580	1583	rVV	3391821	3257582	86.68%	7.010%
28	11.428	1586	1588	1592	rBV	770835	748700	19.92%	1.611%
29	11.886	1663	1666	1668	rVB2	622305	575743	15.32%	1.239%
30	12.575	1779	1783	1786	rVB	3125525	2964446	78.88%	6.379%
31	12.804	1818	1822	1825	rVB	2692291	2916685	77.61%	6.276%
32	12.939	1842	1845	1852	rVB	2756143	2711960	72.16%	5.836%
33	13.986	2019	2023	2026	rBV3	1722787	2382579	63.40%	5.127%
34	14.016	2026	2028	2031	rVB	1397545	1005376	26.75%	2.163%
35	14.192	2056	2058	2065	rVB3	589820	668397	17.78%	1.438%
36	15.021	2194	2199	2202	rBV	1189912	1919734	51.08%	4.131%

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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_F\METHODS\8270-BF100721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.121	2213	2216	2220	rVB	245276	248443	6.61%	0.535%
38	15.316	2245	2249	2255	rVB	731775	940107	25.01%	2.023%
39	15.380	2255	2260	2266	rVV	1001651	1285664	34.21%	2.767%
40	15.439	2266	2270	2273	rVV	857511	1109965	29.53%	2.389%
41	15.468	2273	2275	2281	rVB	419564	471180	12.54%	1.014%
42	16.874	2509	2514	2522	rVB2	373363	713299	18.98%	1.535%
43	17.309	2582	2588	2598	rVB	280917	569617	15.16%	1.226%

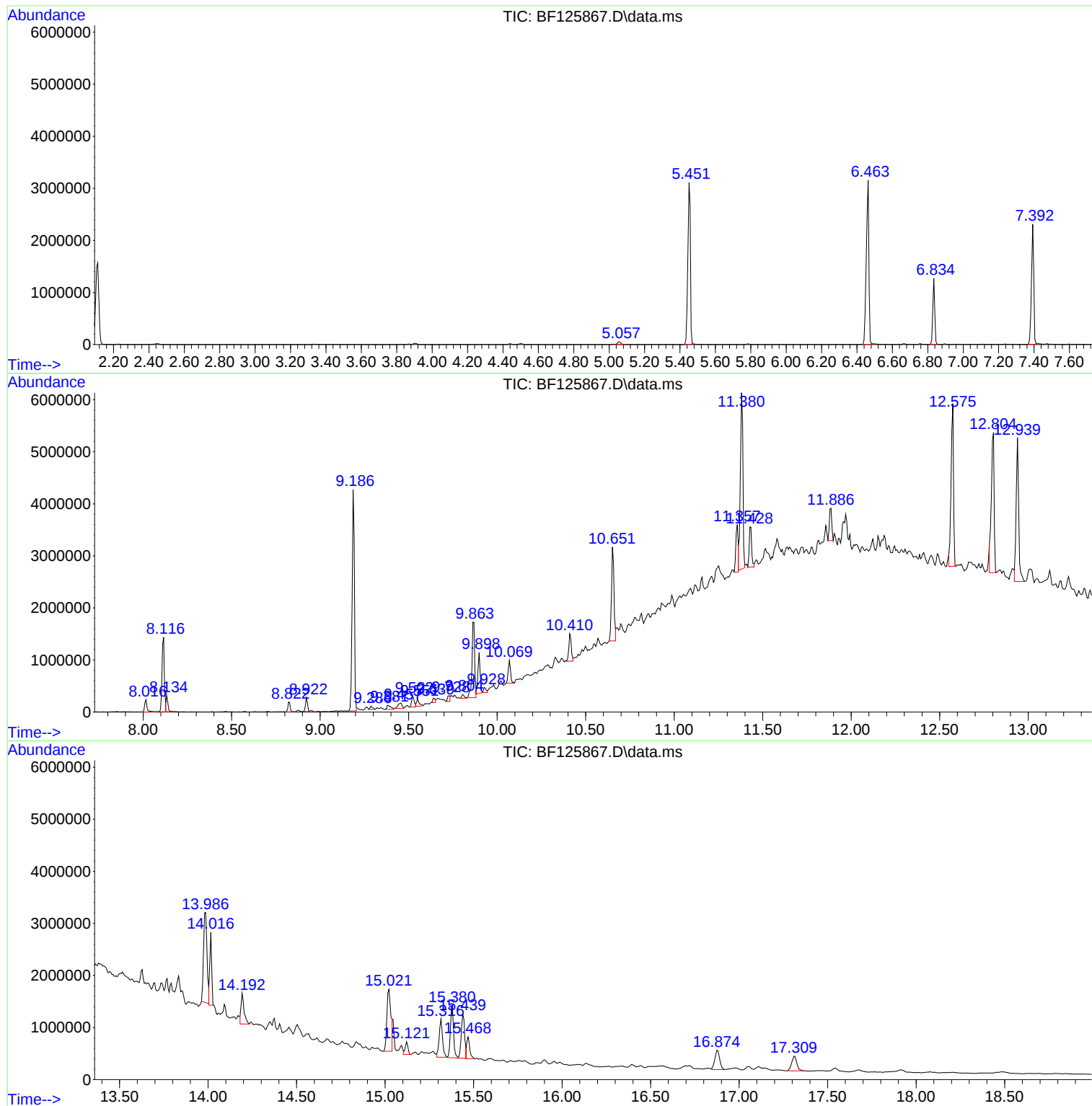
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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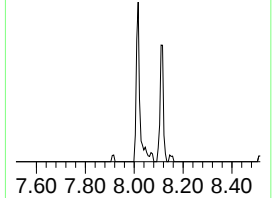
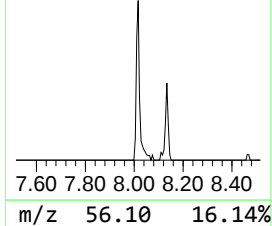
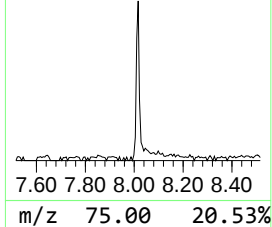
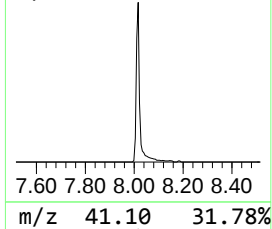
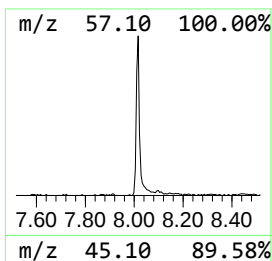
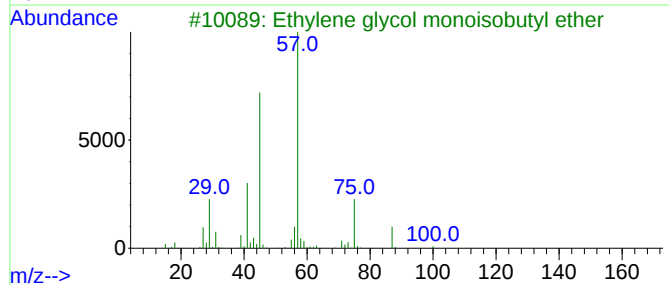
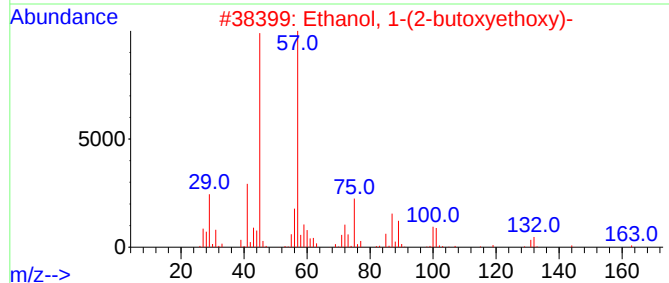
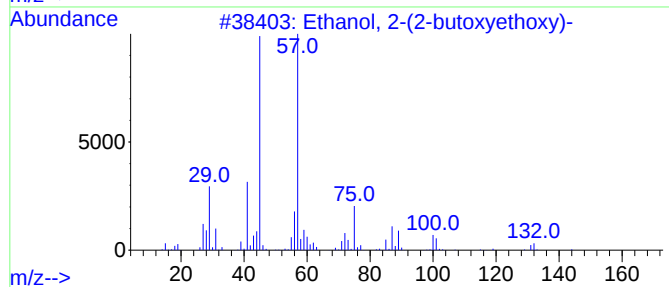
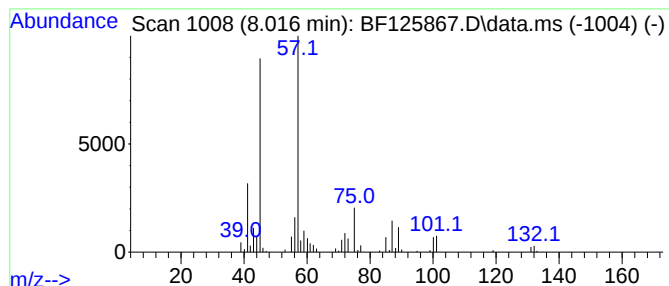
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	3.43 ng	225595	Naphthalene-d8	8.116

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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56



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Instrument :
BNA_F
ClientSampleId :
T3-COMP-(1-4)

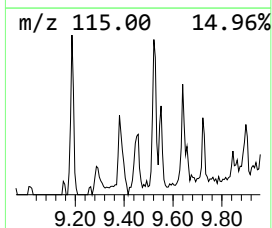
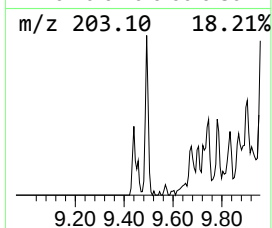
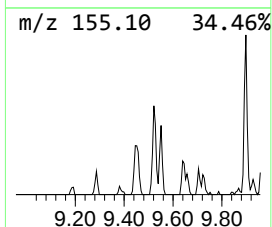
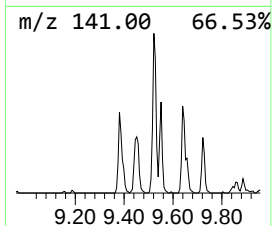
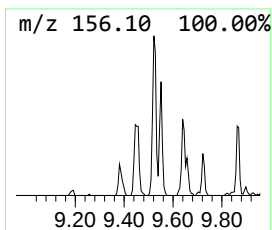
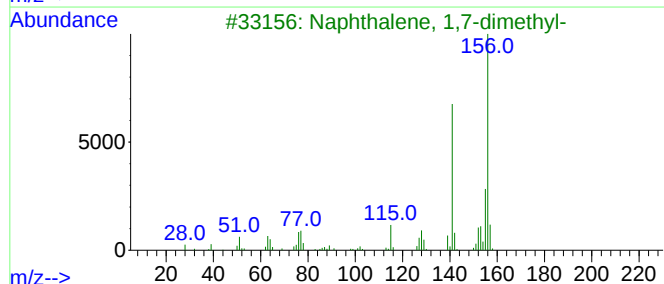
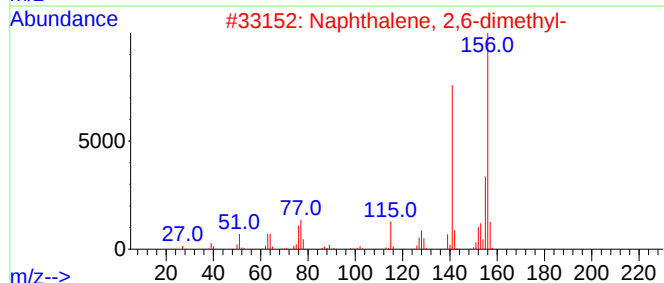
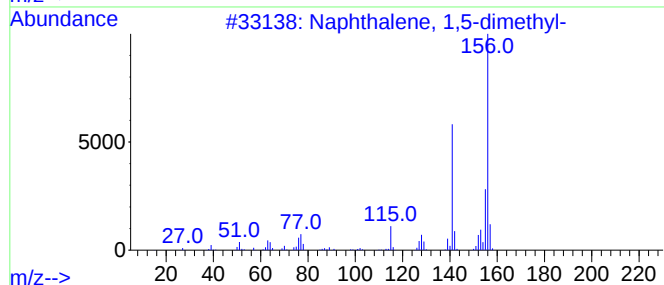
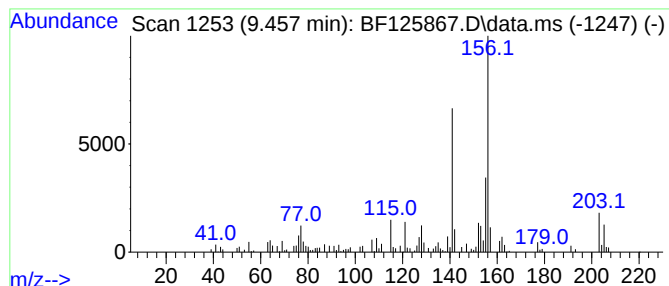
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, 1,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.457	2.13 ng	165741	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
5			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96



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Instrument :
BNA_F
ClientSampleId :
T3-COMP-(1-4)

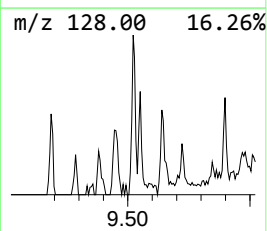
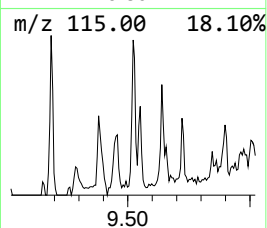
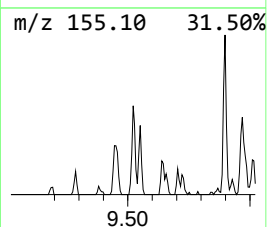
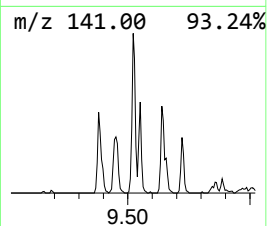
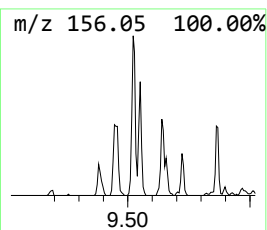
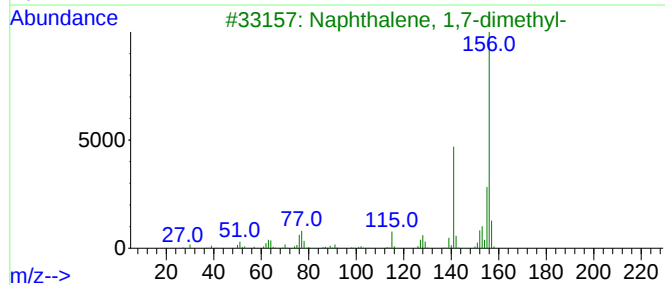
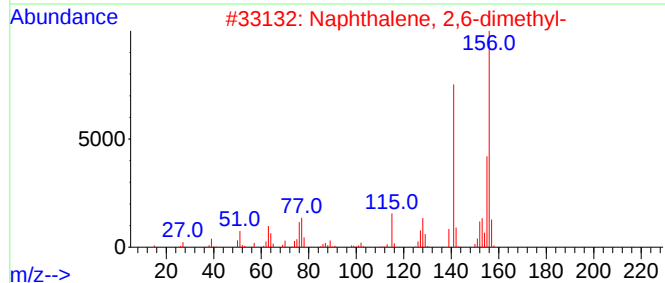
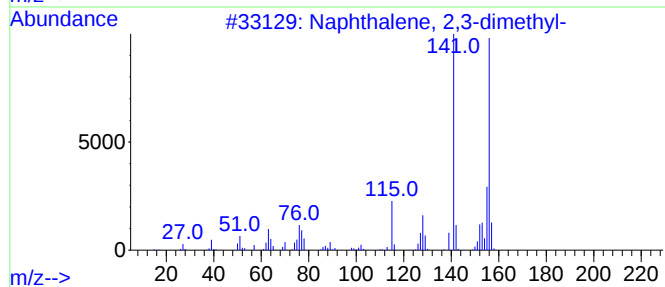
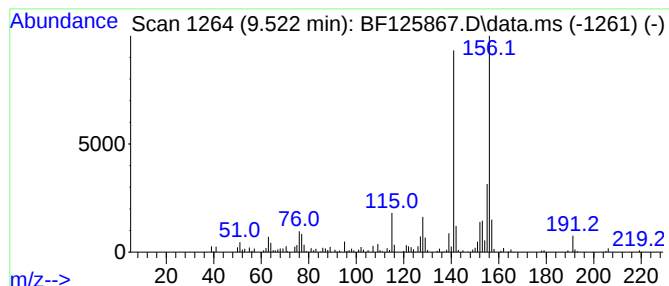
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Naphthalene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.522	2.82 ng	219628	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
5			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96



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Sample : M4243-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T3-COMP-(1-4)

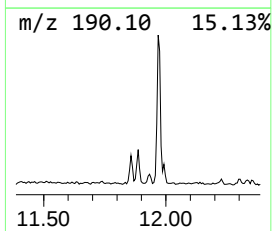
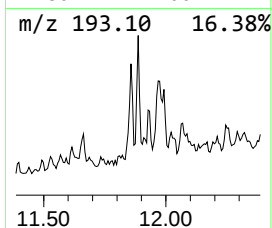
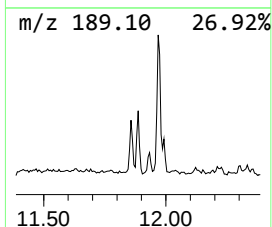
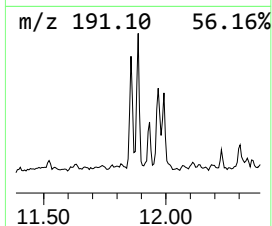
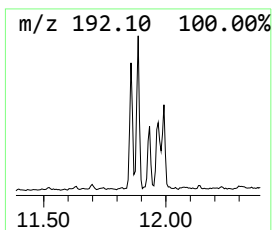
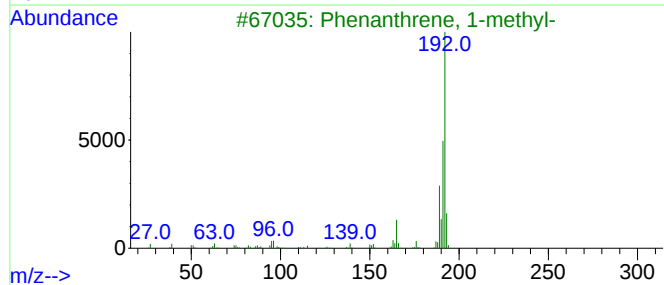
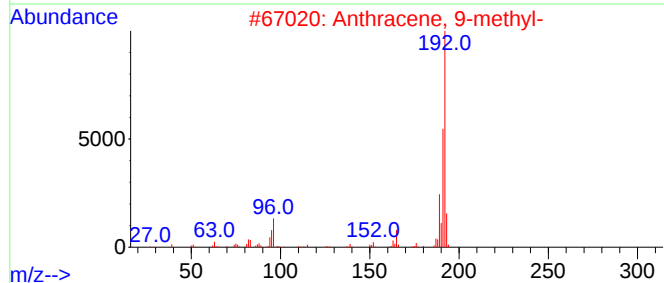
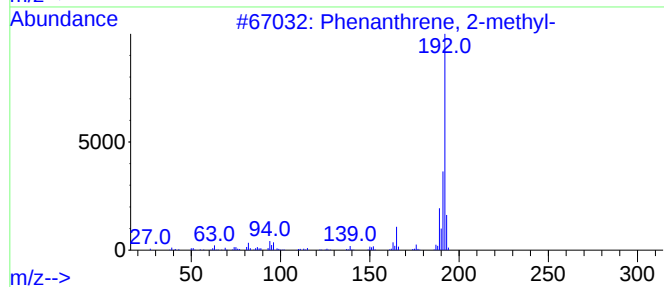
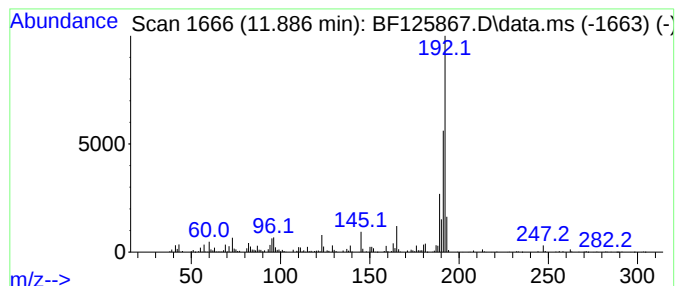
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	13.61 ng	575743	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2			Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	90
4			Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	90



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Instrument :
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T3-COMP-(1-4)

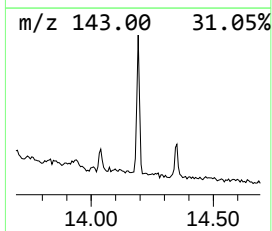
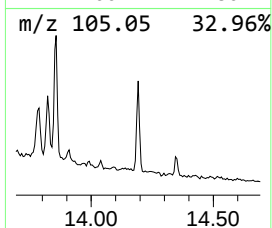
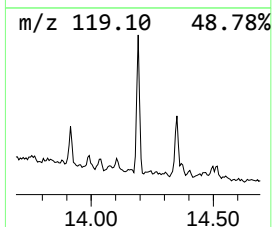
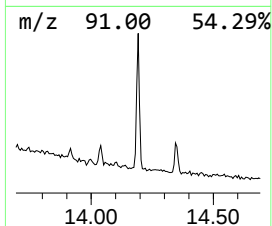
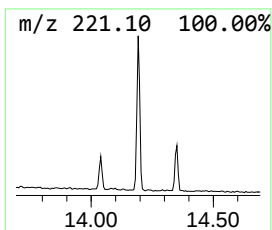
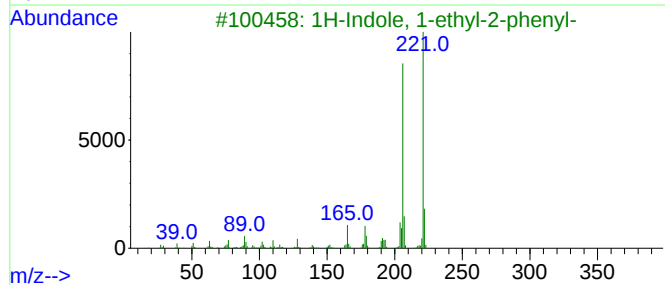
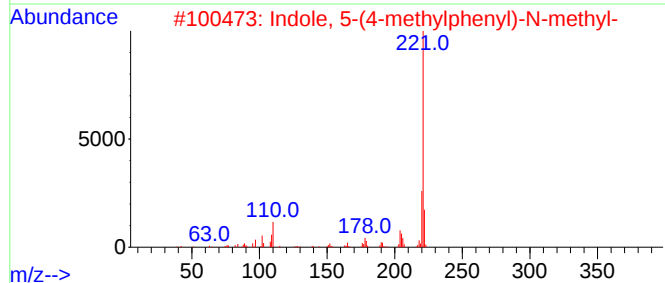
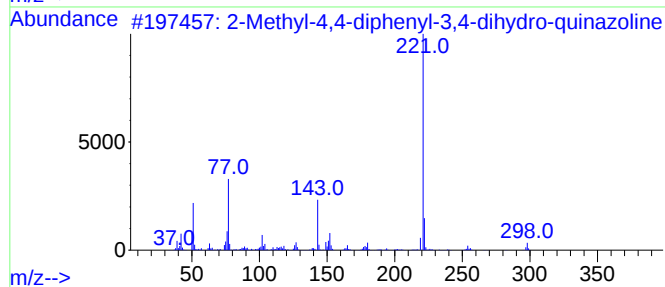
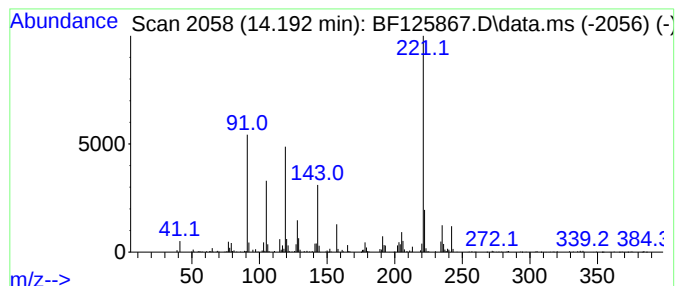
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.192 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	5.61 ng	668397	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-4,4-diphenyl-3,4-dihydr...	298	C21H18N2	1000300-40-0	47
2			Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	43
3			1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	43
4			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	43
5			1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125867.D
Acq On : 15 Oct 2021 17:32
Operator : JU/CG
Sample : M4243-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T3-COMP-(1-4)

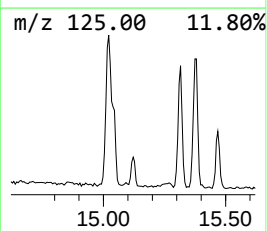
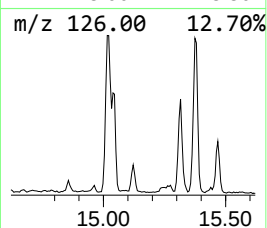
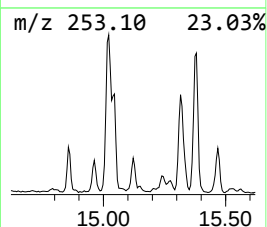
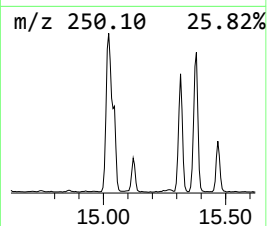
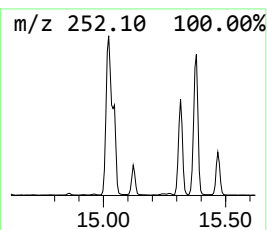
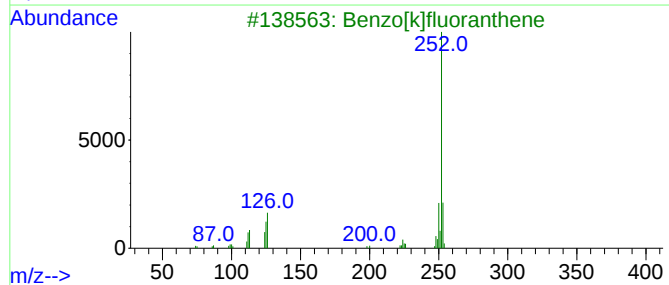
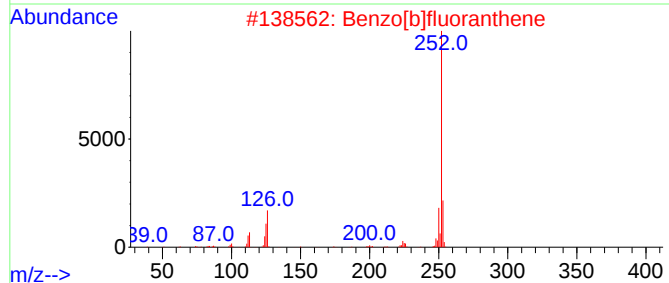
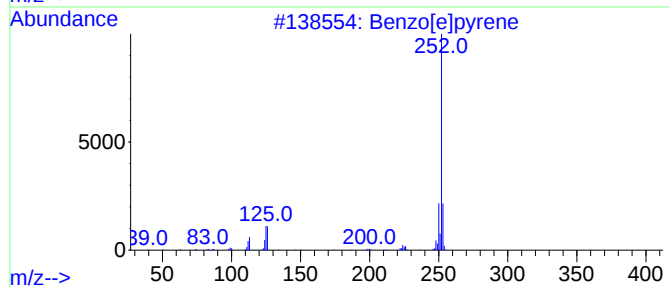
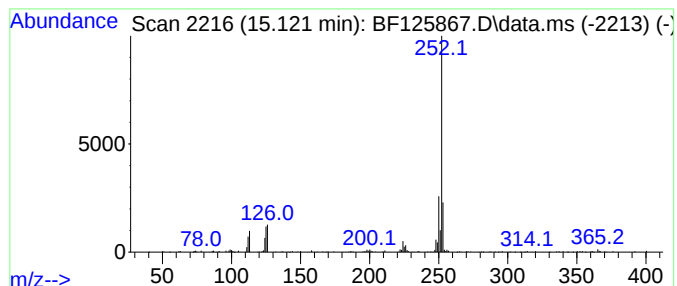
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	4.48 ng	248443	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	93
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4			Benzo[a]pyrene	252	C20H12	000050-32-8	91
5			Perylene	252	C20H12	000198-55-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125867.D
Acq On : 15 Oct 2021 17:32
Operator : JU/CG
Sample : M4243-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T3-COMP-(1-4)

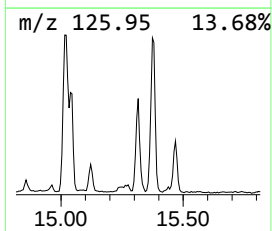
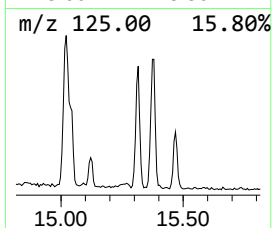
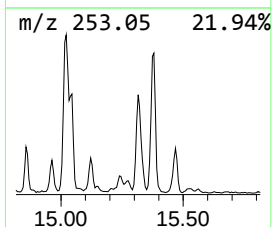
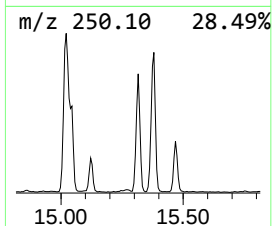
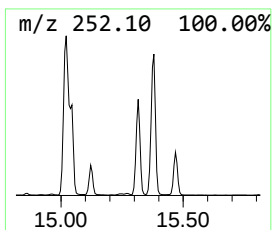
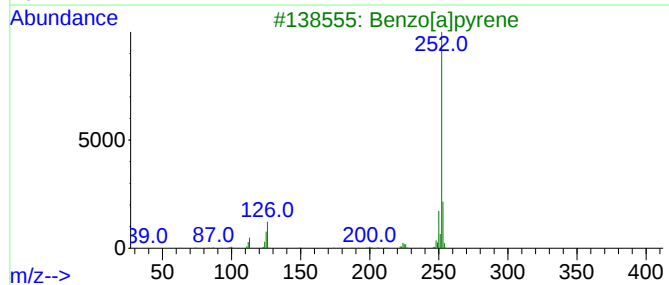
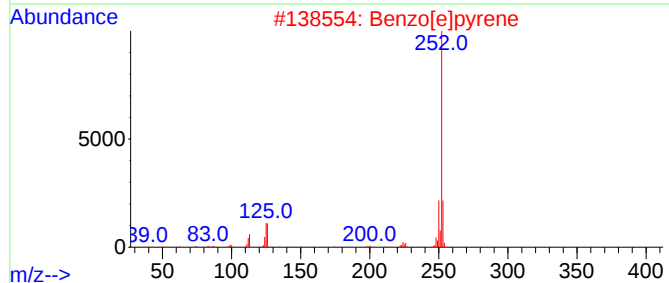
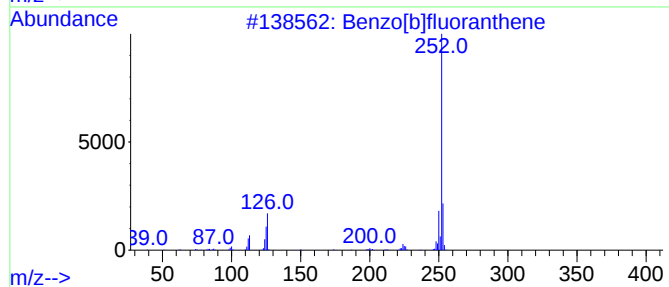
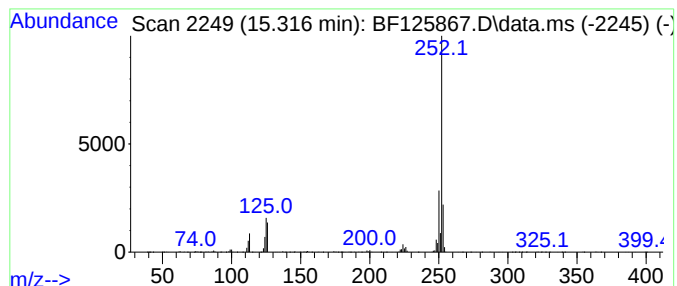
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.316	16.94 ng	940107	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	98
3			Benzo[a]pyrene	252	C20H12	000050-32-8	97
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
5			Perylene	252	C20H12	000198-55-0	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101521\
Data File : BF125867.D
Acq On : 15 Oct 2021 17:32
Operator : JU/CG
Sample : M4243-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T3-COMP-(1-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF100721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	8.016	3.4	ng	225595	2	8.116	1314680	20.0
Naphthalene, 1,...	9.457	2.1	ng	165741	3	9.869	1558370	20.0
Naphthalene, 2,...	9.522	2.8	ng	219628	3	9.869	1558370	20.0
Phenanthrene, 2...	11.886	13.6	ng	575743	4	11.357	845840	20.0
unknown14.192	14.192	5.6	ng	668397	5	13.992	2382580	20.0
Benzo[e]pyrene	15.121	4.5	ng	248443	6	15.439	1109970	20.0
Perylene	15.316	16.9	ng	940107	6	15.439	1109970	20.0