LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133852.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	15	rVB	284511	356892	28.16%	2.650%
2	2.240	24	26	34	rVB3	14510	21169	1.67%	0.157%
3	5.081	506	509	517	rVB	70152	77248	6.09%	0.573%
4	5.487	574	578	591	rVB	1154579	1034710	81.63%	7.682%
5	6.493	745	749	759	rBV	1113156	1019341	80.42%	7.568%
6	6.857	807	811	814	rBV	739831	570462	45.01%	4.235%
7	7.416	902	906	909	rBV	853255	665263	52.49%	4.939%
8	8.134	1025	1028	1036	rVB	845958	727396	57.39%	5.400%
9	8.851	1146	1150	1154	rVB	17350	16763	1.32%	0.124%
10	9.210	1208	1211	1215	rBV	1575040	1267484	100.00%	9.410%
11	9.751	1301	1303	1307	rBV	27643	24581	1.94%	0.182%
12	9.892	1324	1327	1331	rBV	862770	696550	54.96%	5.171%
13	9.928	1331	1333	1340	rVB	28080	26008	2.05%	0.193%
14	10.098	1358	1362	1367	rBV	30016	29953	2.36%	0.222%
15	10.439	1417	1420	1425	rBV3	20736	22827	1.80%	0.169%
16	10.610	1444	1449	1452	rBV	264739	222222	17.53%	1.650%
17	10.686	1458	1462	1466	rBV	662790	599684	47.31%	4.452%
18	10.810	1478	1483	1489	rBV3	24310	37017	2.92%	0.275%
19	10.922	1500	1502	1505	rVB	27396	20113	1.59%	0.149%
20	11.192	1545	1548	1553	rBV3	15134	15692	1.24%	0.116%
21	11.280	1561	1563	1568	rVB	21571	20831	1.64%	0.155%
22	11.386	1577	1581	1583	rBV	739304	598965	47.26%	4.447%
23	11.410	1583	1585	1589	rVV	227296	182249	14.38%	1.353%
24	11.463	1591	1594	1597	rVB	53852	48171	3.80%	0.358%
25	11.622	1618	1621	1624	rBV	18140	20655	1.63%	0.153%
26	11.686	1628	1632	1636	rBV5	18007	21451	1.69%	0.159%
27	11.845	1657	1659	1662	rBV4	12419	16716	1.32%	0.124%
28	11.892	1664	1667	1669	rVV	46449	53971	4.26%	0.401%
29	11.922	1669	1672	1682	rVB2	186185	273233	21.56%	2.029%
30	12.004	1683	1686	1688	rBV2	53612	52369	4.13%	0.389%
31	12.186	1715	1717	1720	rBV	28131	29153	2.30%	0.216%
32	12.216	1720	1722	1725	rVB2	26447	20526	1.62%	0.152%
33	12.445	1758	1761	1764	rBV2	30577	33770	2.66%	0.251%
34	12.527	1773	1775	1780	rBV2	29178	34453	2.72%	0.256%
35	12.610	1785	1789	1792	rBV	362590	349220	27.55%	2.593%
36	12.663	1793	1798	1802	rVV4	82947	161322	12.73%	1.198%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.710	1803	1806	1813	rVB3	81957	132494	10.45%	0.984%
38	12.839	1822	1828	1830	rBV	395149	373919	29.50%	2.776%
39	12.980	1849	1852	1856	rVB	1009644	880165	69.44%	6.534%
40	13.145	1877	1880	1881	rBV2	25035	27019	2.13%	0.201%
41	13.169	1882	1884	1886	rVB	48824	40662	3.21%	0.302%
42	13.233	1893	1895	1898	rVB	40665	33808	2.67%	0.251%
43	13.274	1898	1902	1904	rBV2	43849	54540	4.30%	0.405%
44	13.363	1915	1917	1920	rVB	29776	26256	2.07%	0.195%
45	13.398	1921	1923	1927	rVB	32533	30553	2.41%	0.227%
46	13.680	1968	1971	1975	rVB	40493	41939	3.31%	0.311%
47	13.892	2004	2007	2009	rBV3	47094	43486	3.43%	0.323%
48	14.045	2028	2033	2036	rBV2	706002	881337	69.53%	6.543%
49	14.069	2036	2037	2043	rVB	224069	178284	14.07%	1.324%
50	14.151	2049	2051	2053	rVB2	53049	38238	3.02%	0.284%
51	15.104	2209	2213	2217	rBV	266793	424503	33.49%	3.152%
52	15.421	2264	2267	2272	rVB	129230	152010	11.99%	1.129%
53	15.486	2275	2278	2283	rBV	171703	208687	16.46%	1.549%
54	15.551	2285	2289	2293	rBV	400498	533331	42.08%	3.959%

Sum of corrected areas: 13469661

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
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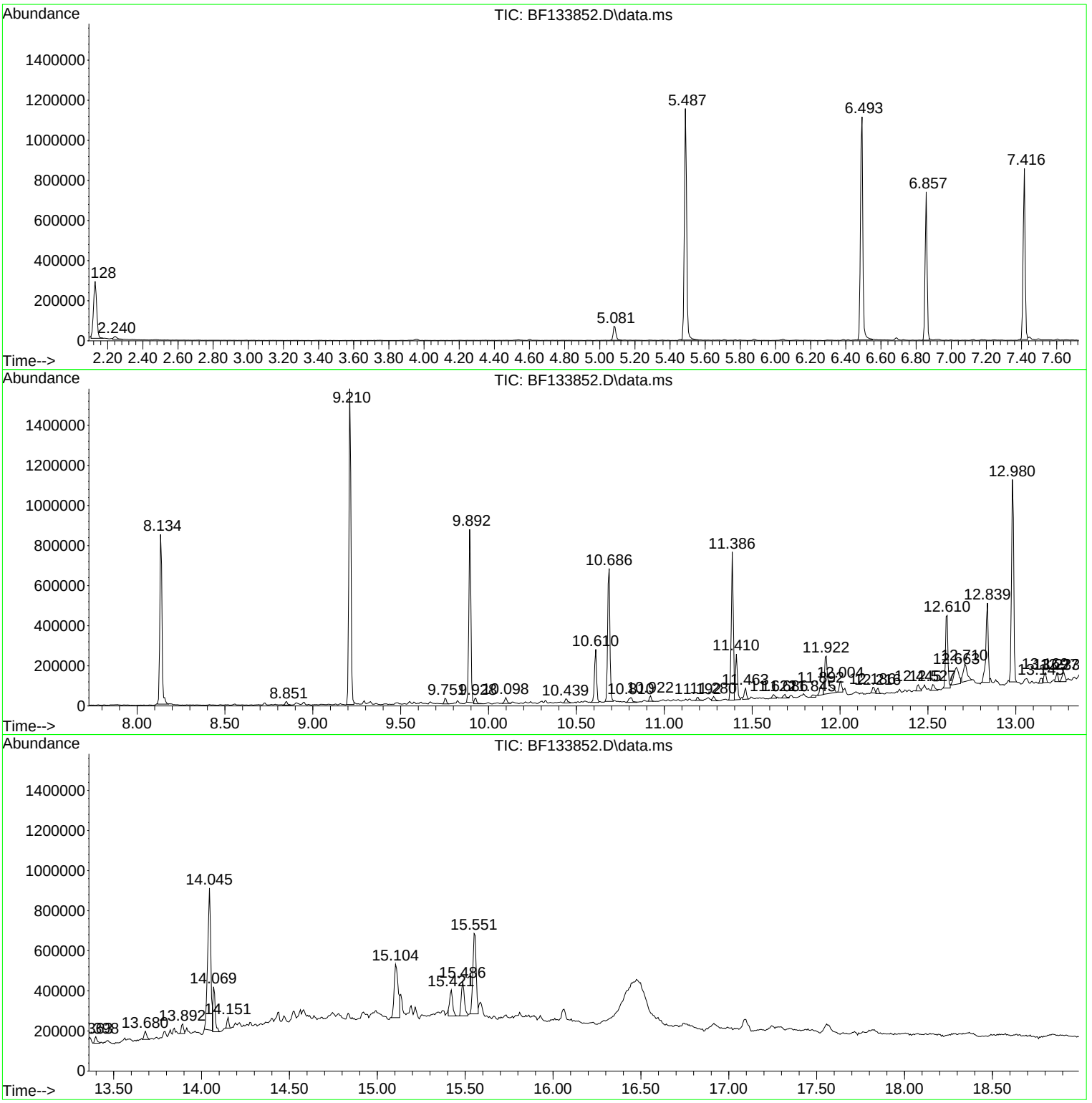
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

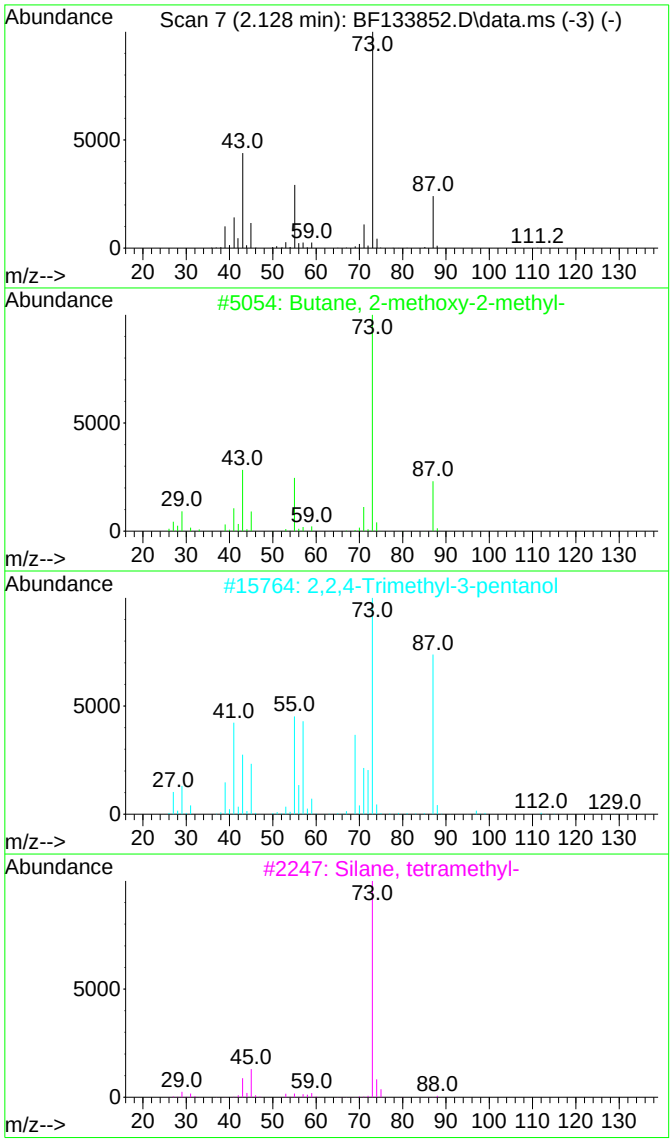
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

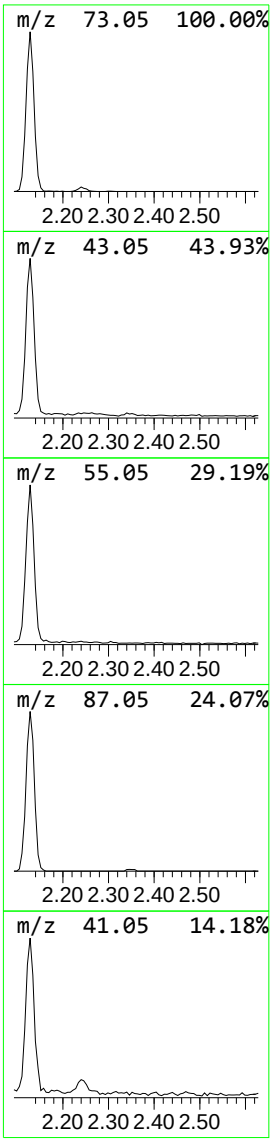
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	12.51 ng	356892	1,4-Dichlorobenzene-d4	6.857

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

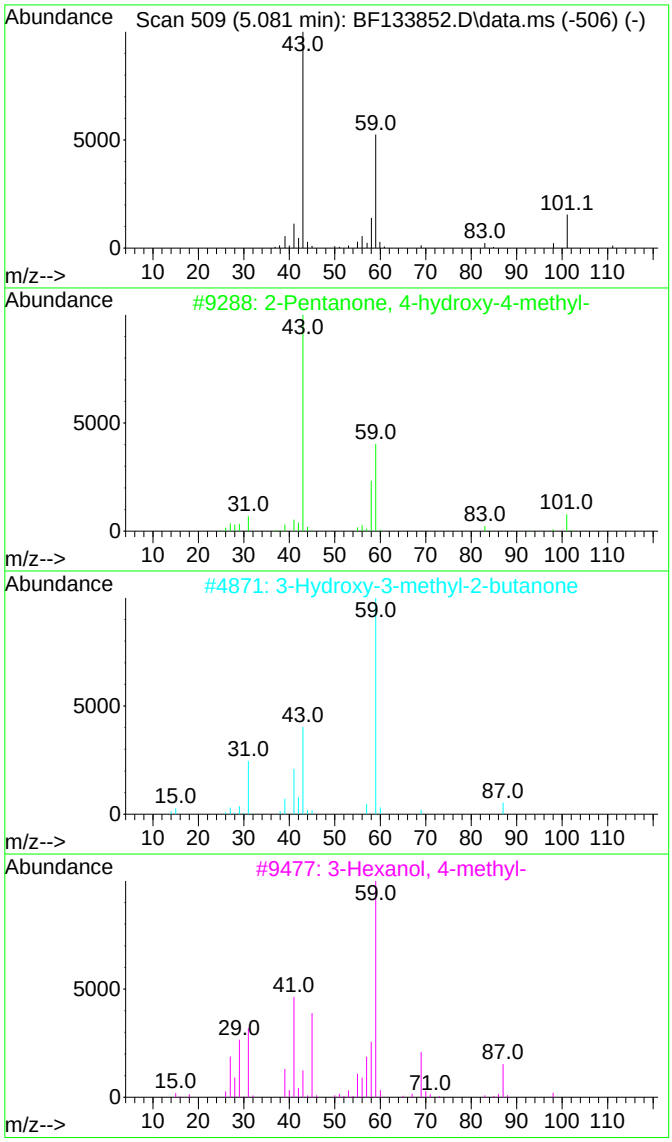
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

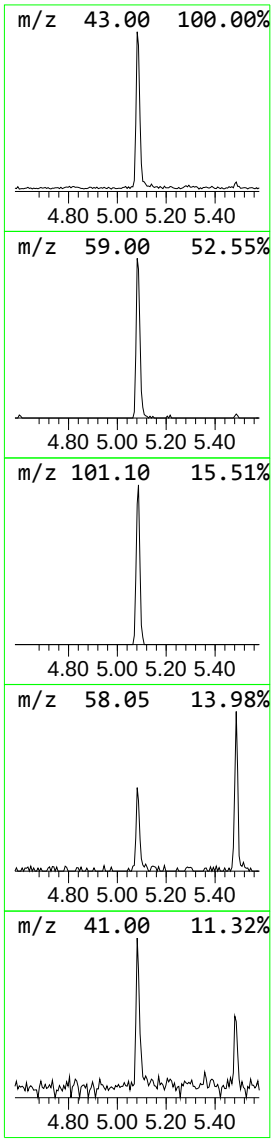
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	2.71 ng	77248	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	14
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

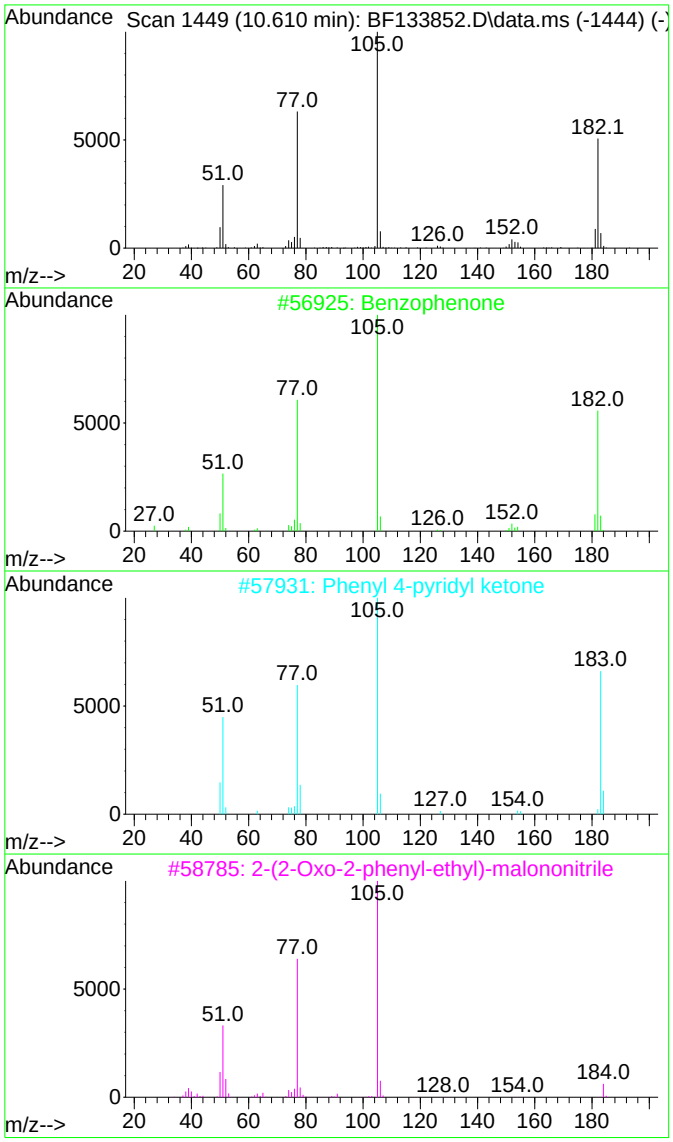
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

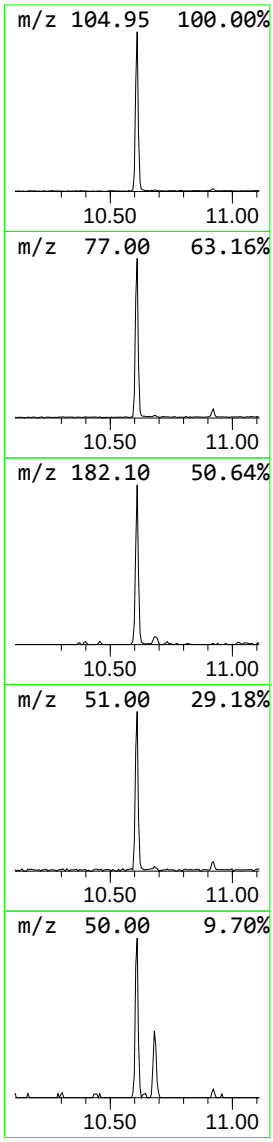
****

Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	6.38 ng	222222	Acenaphthene-d10	9.892

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

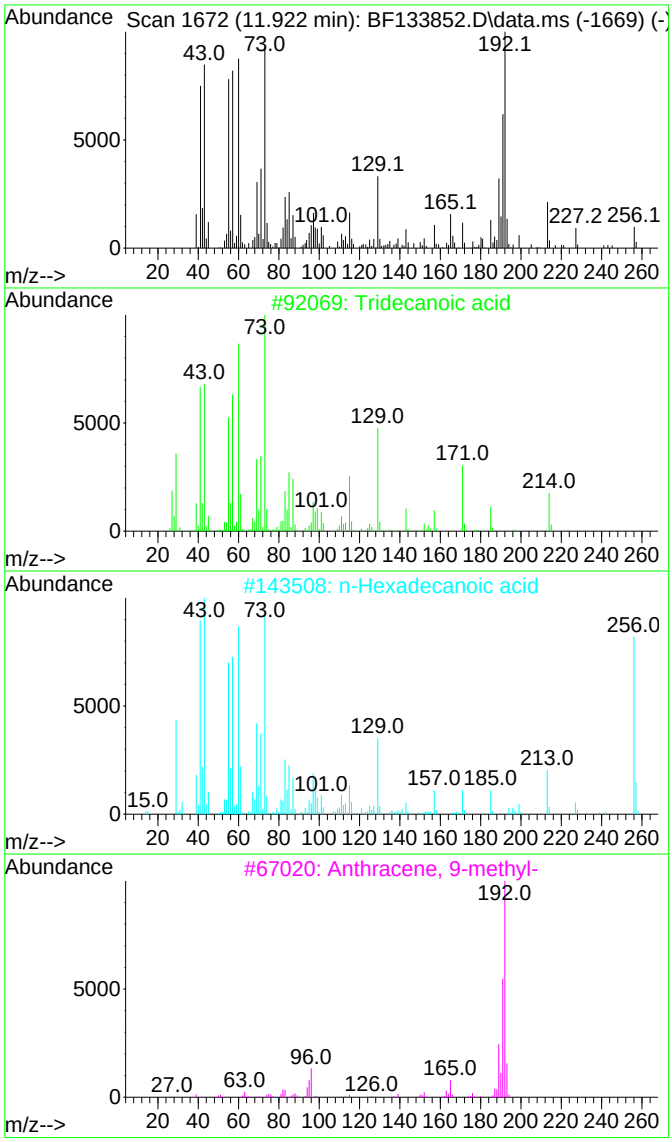
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

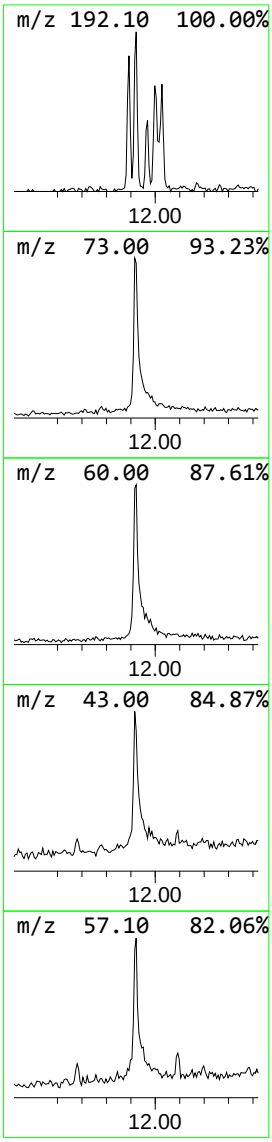
****

Peak Number 4 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	9.12 ng	273233	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	84
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	78
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

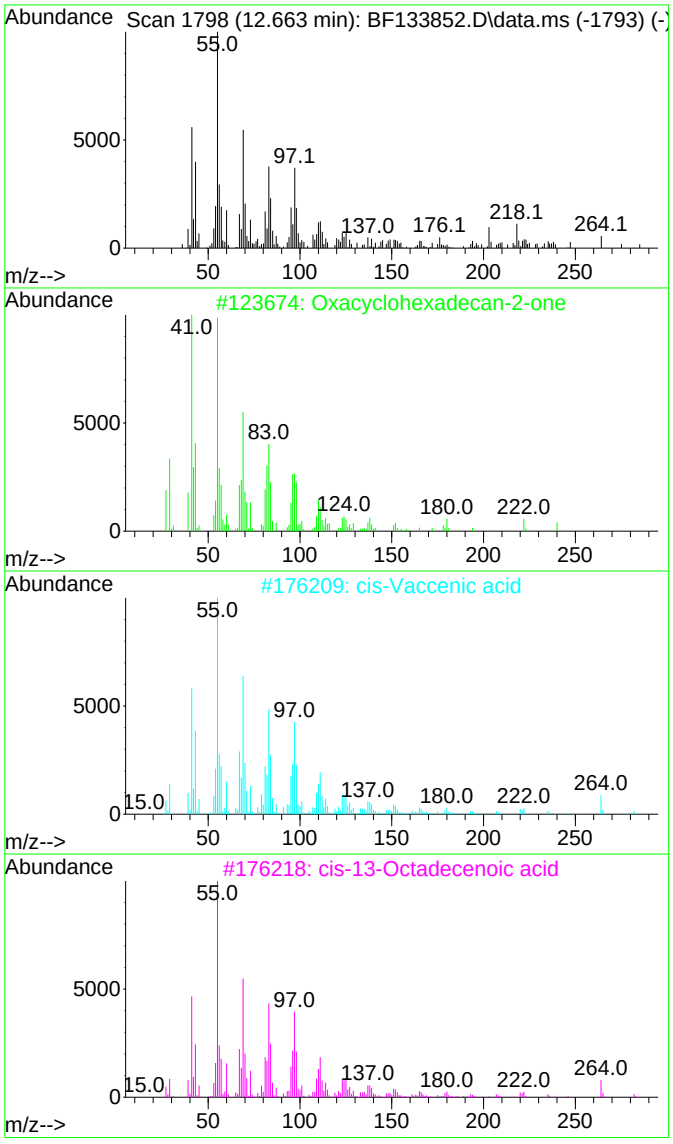
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

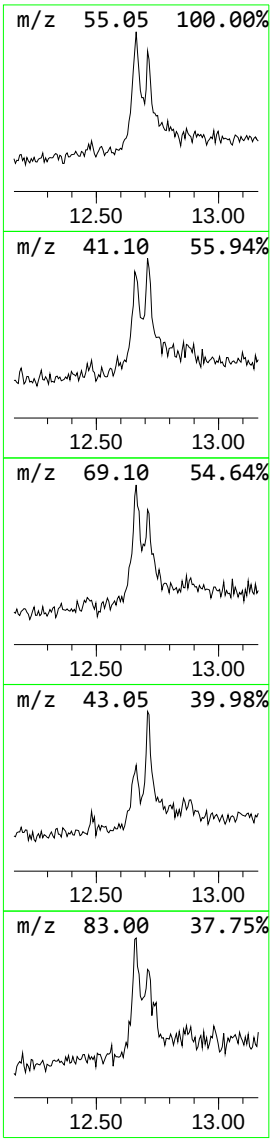
****

Peak Number 5 Oxacyclohexadecan-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.663	5.39 ng	161322	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxacyclohexadecan-2-one	240	C15H28O2	000106-02-5	64
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	64
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	64
4	Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	52
5	Cyclopropane, nonyl-	168	C12H24	074663-85-7	46





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Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

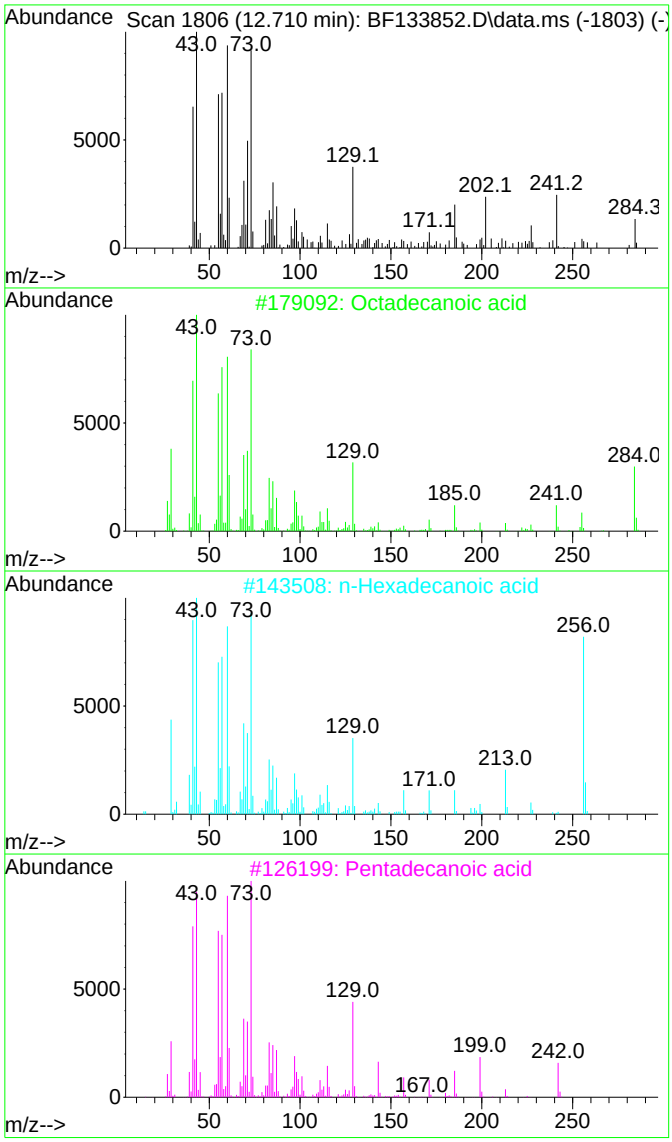
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

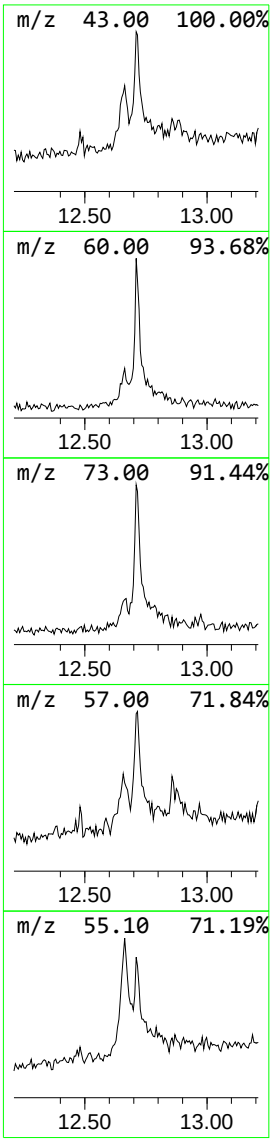
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	4.42 ng	132494	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

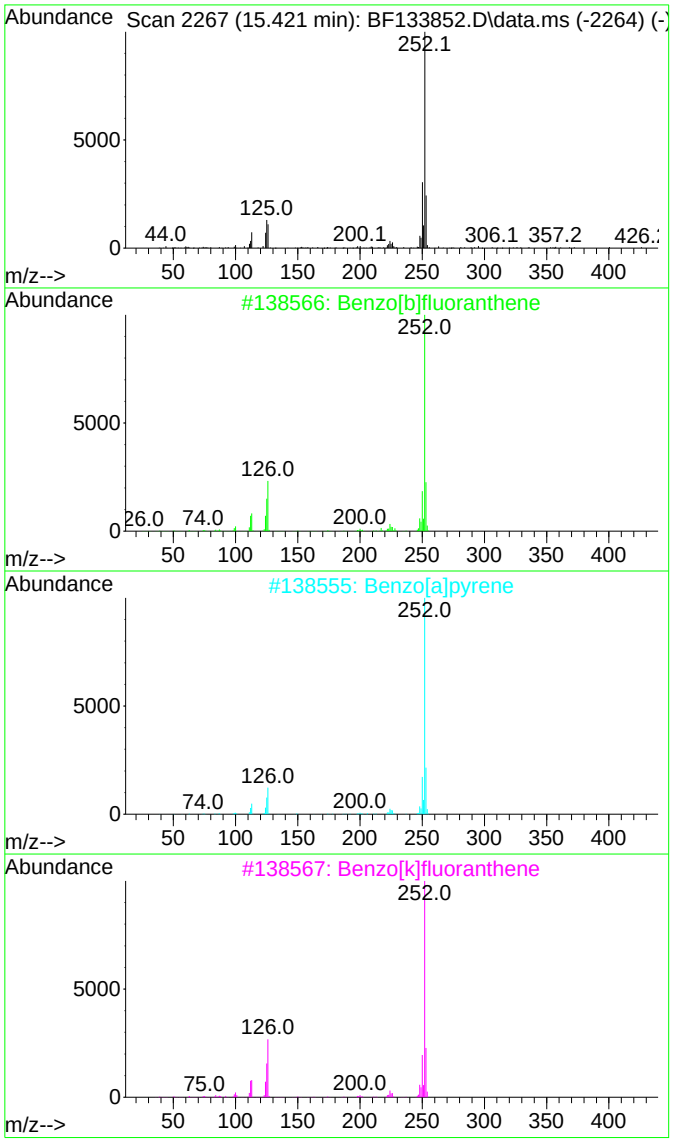
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

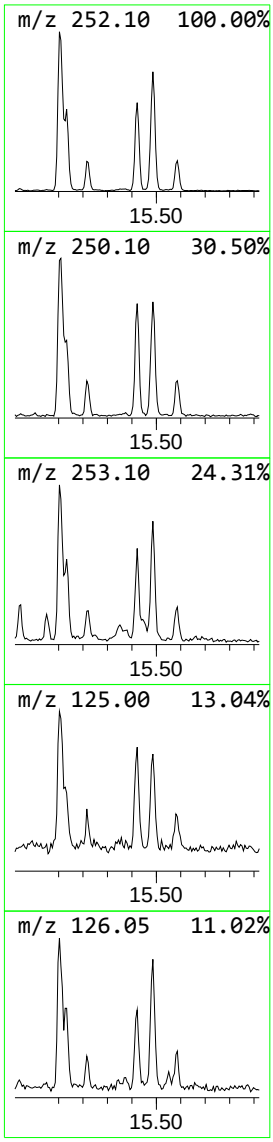
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.421	5.70 ng	152010	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	92
4	Benzo[e]pyrene	252	C20H12	000192-97-2	91
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133852.D
Acq On : 20 Jun 2023 12:52
Operator : CG\JU
Sample : 03222-13 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-SB-06

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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...	2.128	12.5	ng	356892	1	6.857	570462	20.0
2-Pentanone, 4-...	5.081	2.7	ng	77248	1	6.857	570462	20.0
Benzophenone	10.610	6.4	ng	222222	3	9.892	696550	20.0
Tridecanoic acid	11.922	9.1	ng	273233	4	11.386	598965	20.0
Oxacyclohexadec...	12.663	5.4	ng	161322	4	11.386	598965	20.0
Octadecanoic acid	12.710	4.4	ng	132494	4	11.386	598965	20.0
Benzo[e]pyrene	15.421	5.7	ng	152010	6	15.551	533331	20.0