LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11995

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131136.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	8	15	21	rBV	516843	690713	36.24%	4.494%
2	2.287	29	34	41	rBV	40103	53231	2.79%	0.346%
3	5.116	510	515	524	rBV	263575	335308	17.59%	2.182%
4	5.510	577	582	585	rBV	2047660	1846014	96.86%	12.011%
5	6.516	748	753	756	rBV	1869951	1837828	96.43%	11.958%
6	6.887	813	816	820	rBV	553083	427205	22.42%	2.780%
7	7.451	907	912	915	rBV	1213622	1201396	63.04%	7.817%
8	8.175	1030	1035	1038	rBV	580241	539358	28.30%	3.509%
9	9.251	1213	1218	1221	rBV	2176234	1905771	100.00%	12.400%
10	9.933	1330	1334	1337	rBV	587364	527162	27.66%	3.430%
11	10.722	1464	1468	1477	rBV	1073956	922435	48.40%	6.002%
12	11.422	1584	1587	1590	rBV	493487	426384	22.37%	2.774%
13	11.445	1590	1591	1595	rVB	85883	55301	2.90%	0.360%
14	12.039	1688	1692	1694	rBV2	20107	22133	1.16%	0.144%
15	12.639	1791	1794	1798	rBV	263711	210323	11.04%	1.368%
16	12.868	1828	1833	1837	rBV	220286	240304	12.61%	1.564%
17	13.010	1853	1857	1861	rBV	1505129	1379470	72.38%	8.975%
18	13.086	1866	1870	1874	rBV2	21201	36419	1.91%	0.237%
19	13.198	1887	1889	1892	rVB	38113	34601	1.82%	0.225%
20	13.263	1898	1900	1903	rBV	24883	22380	1.17%	0.146%
21	13.304	1903	1907	1909	rVV2	30777	35967	1.89%	0.234%
22	13.574	1950	1953	1956	rBV4	19415	22196	1.16%	0.144%
23	13.710	1973	1976	1981	rVB	33650	33904	1.78%	0.221%
24	13.821	1990	1995	1998	rBV3	36944	49492	2.60%	0.322%
25	13.874	2002	2004	2007	rVV2	29290	36878	1.94%	0.240%
26	13.915	2007	2011	2015	rVV2	35857	49299	2.59%	0.321%
27	13.980	2015	2022	2030	rVV4	46644	156745	8.22%	1.020%
28	14.074	2030	2038	2040	rVV2	528125	627294	32.92%	4.081%
29	14.098	2040	2042	2049	rVB	172552	147815	7.76%	0.962%
30	14.168	2049	2054	2058	rBV2	61169	93815	4.92%	0.610%
31	14.457	2099	2103	2106	rVB	37356	40096	2.10%	0.261%
32	14.492	2107	2109	2113	rVB2	23072	26314	1.38%	0.171%
33	14.527	2113	2115	2117	rBV	28103	25177	1.32%	0.164%
34	14.586	2122	2125	2127	rBV2	23105	24680	1.30%	0.161%
35	15.127	2213	2217	2220	rBV	190030	266418	13.98%	1.733%
36	15.192	2225	2228	2233	rVB5	31422	43050	2.26%	0.280%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.239	2233	2236	2239	rBV	26421	27202	1.43%	0.177%
38	15.439	2267	2270	2276	rVB	108112	129170	6.78%	0.840%
39	15.504	2277	2281	2286	rBV	125163	159556	8.37%	1.038%
40	15.568	2287	2292	2297	rBV	303210	408496	21.43%	2.658%
41	16.027	2367	2370	2374	rVB4	18338	25175	1.32%	0.164%
42	16.727	2487	2489	2496	rVB6	31437	54705	2.87%	0.356%
43	17.074	2544	2548	2556	rVB2	41708	83421	4.38%	0.543%
44	17.333	2588	2592	2598	rVB7	14156	23154	1.21%	0.151%
45	17.539	2622	2627	2634	rVB2	32684	65550	3.44%	0.426%

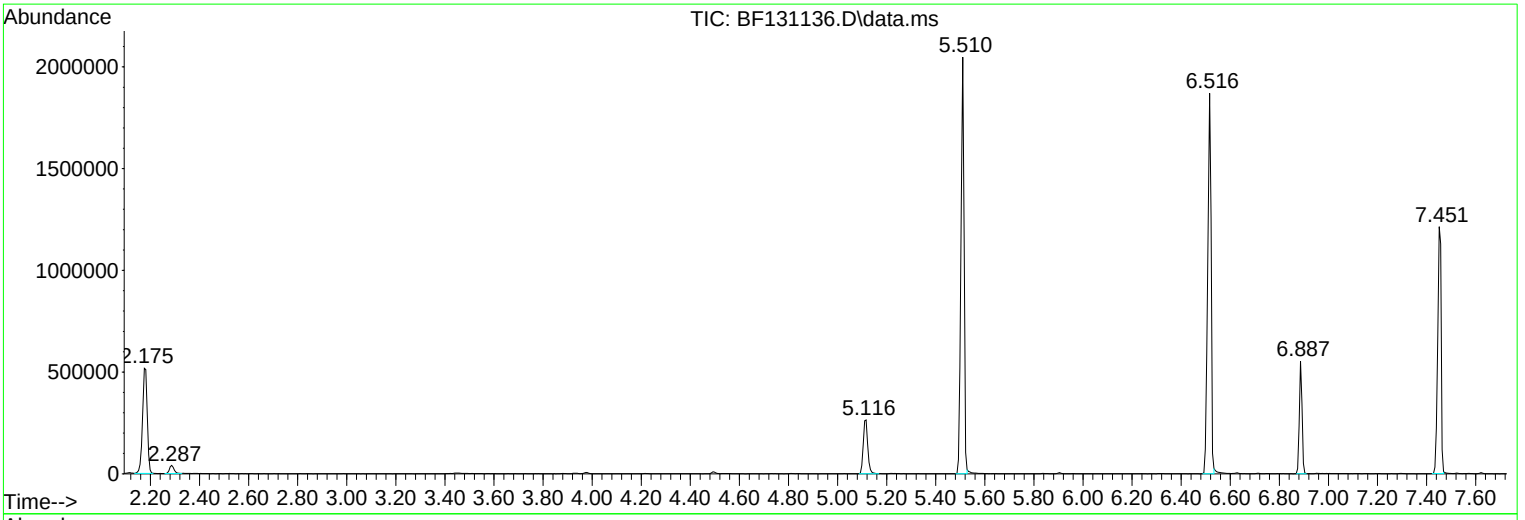
Sum of corrected areas: 15369305

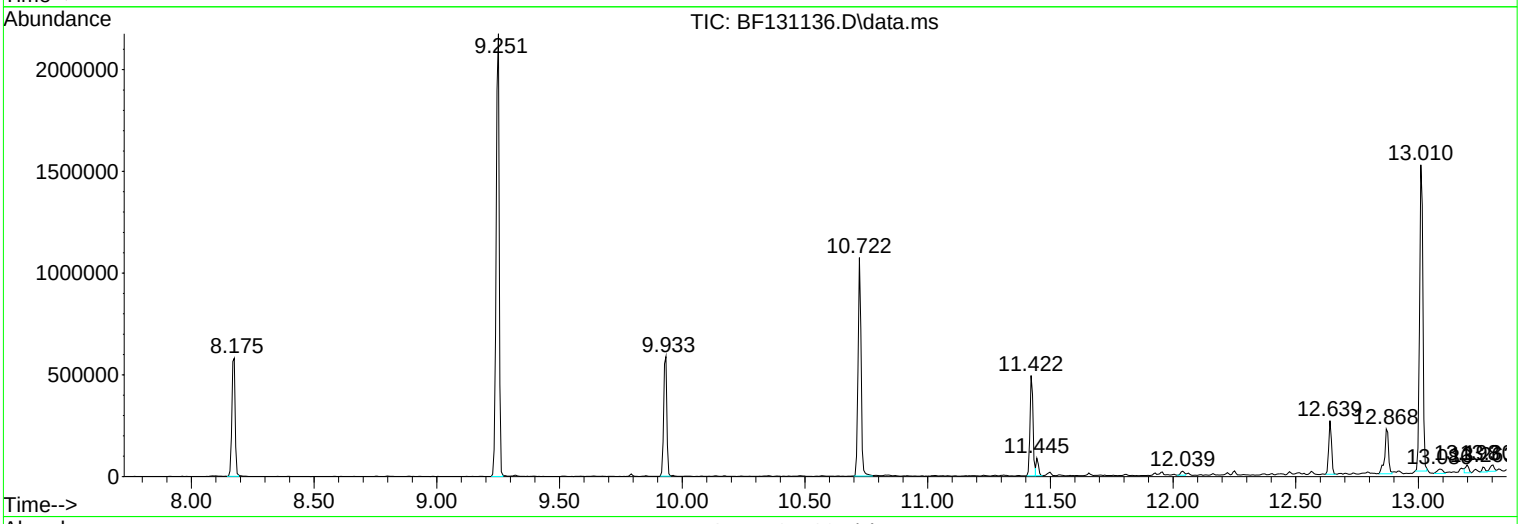
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

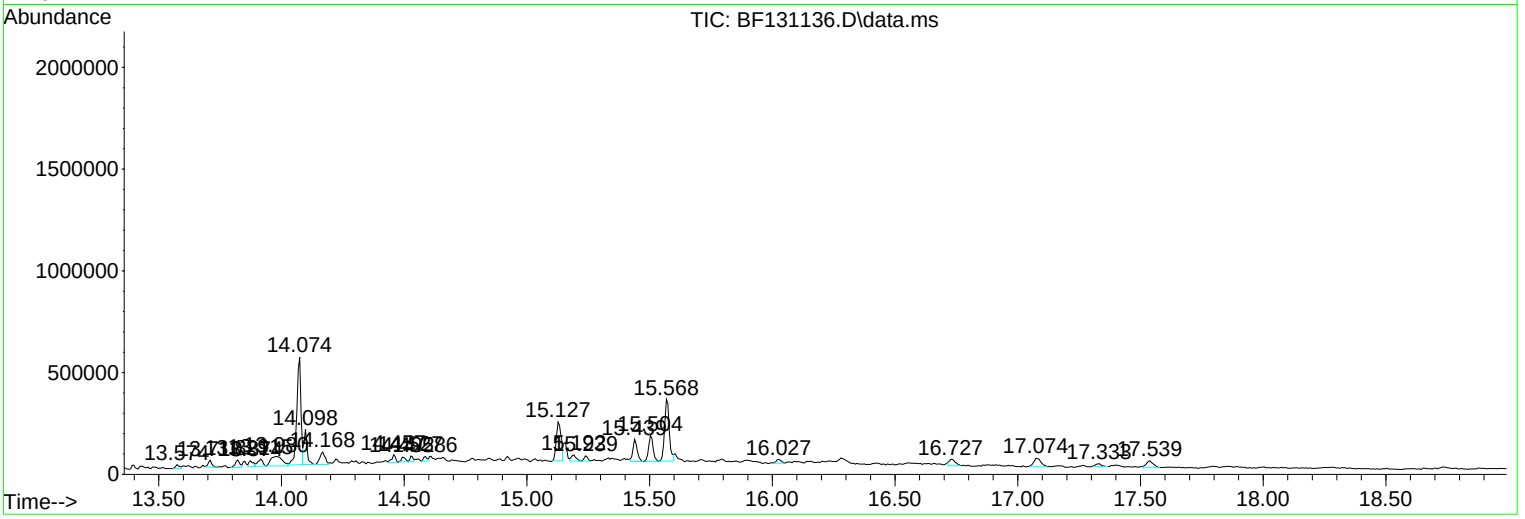
Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

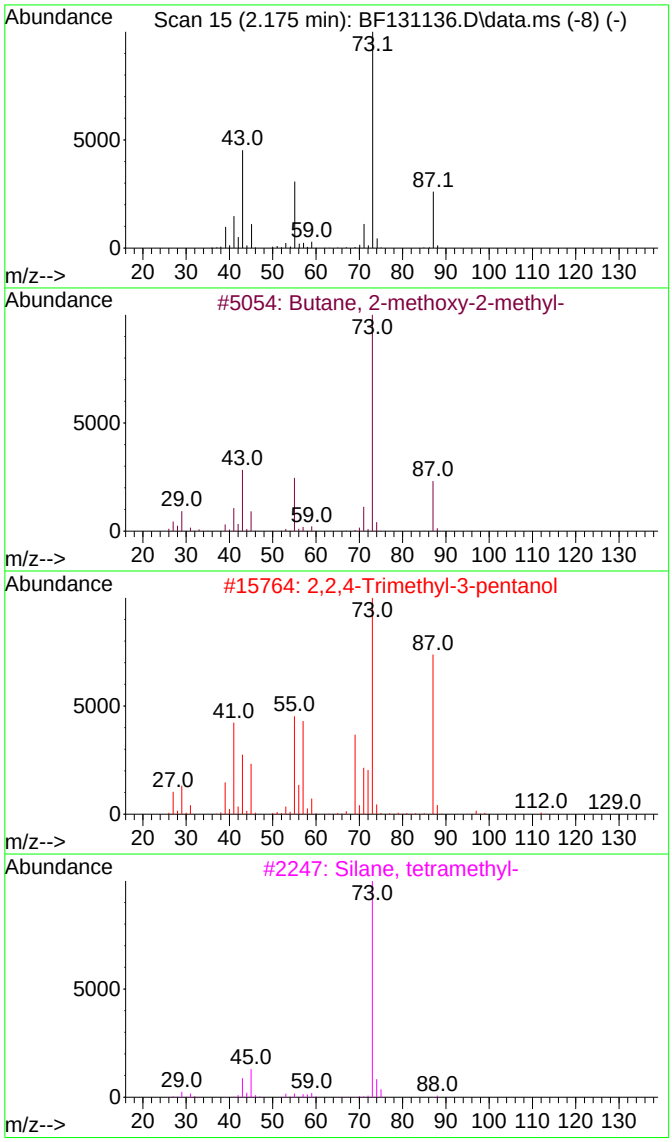
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

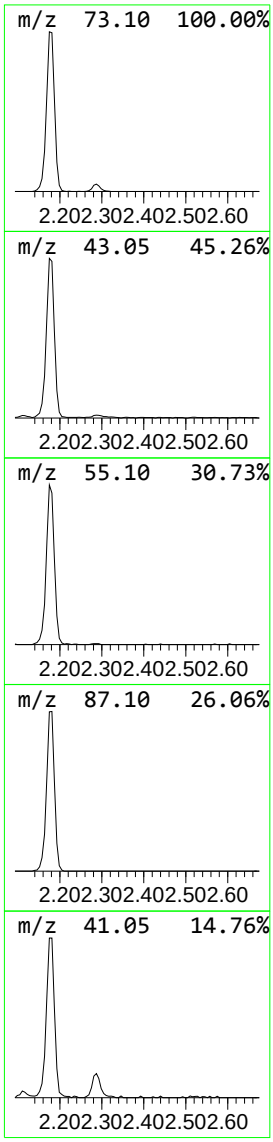
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	32.34 ng	690713	1,4-Dichlorobenzene-d4	6.886

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	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
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Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

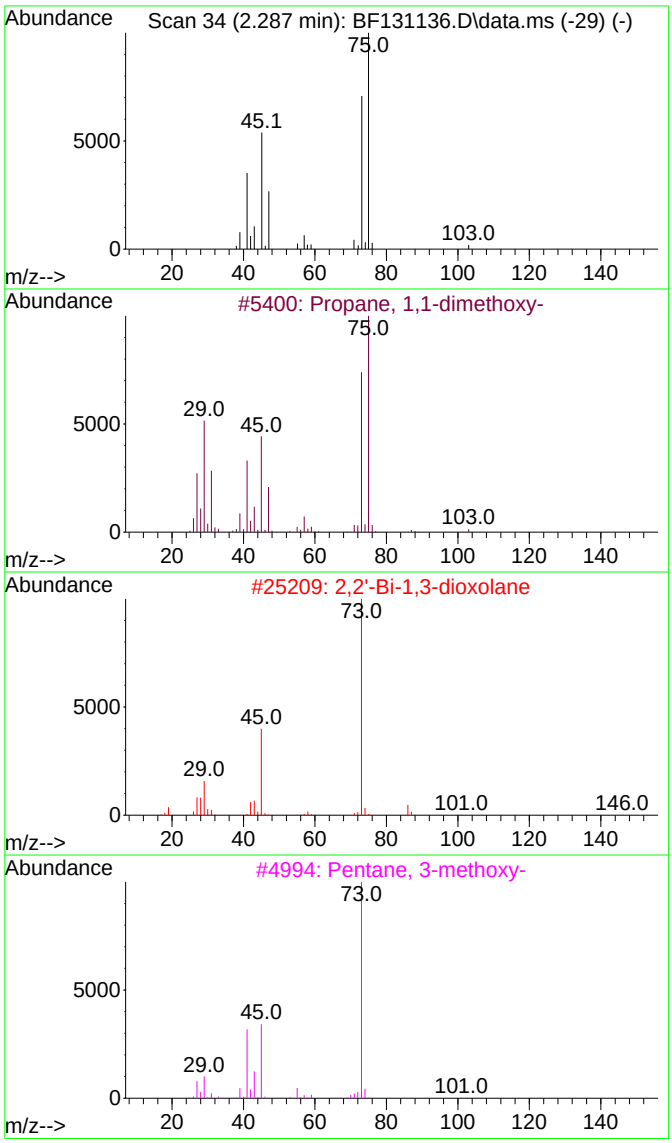
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

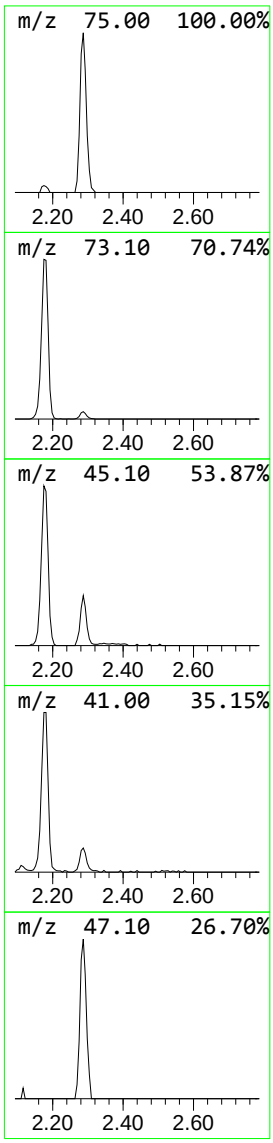
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	2.49 ng	53231	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	14
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	1-Butanol, 4-methoxy-	104	C5H12O2	000111-32-0	10
5	3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

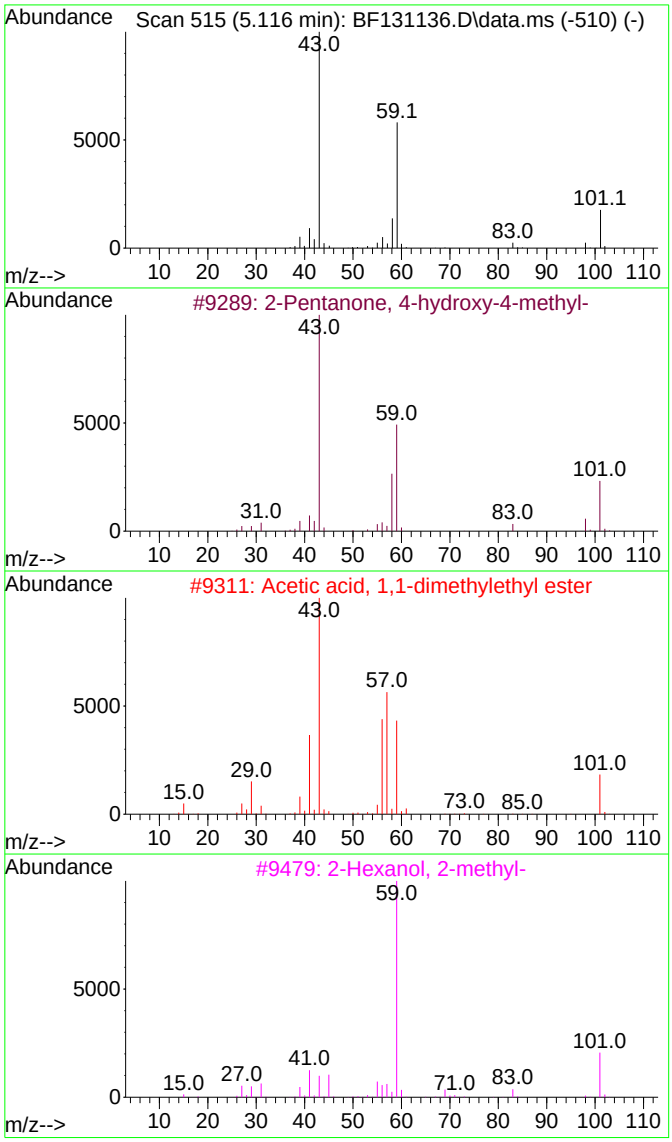
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

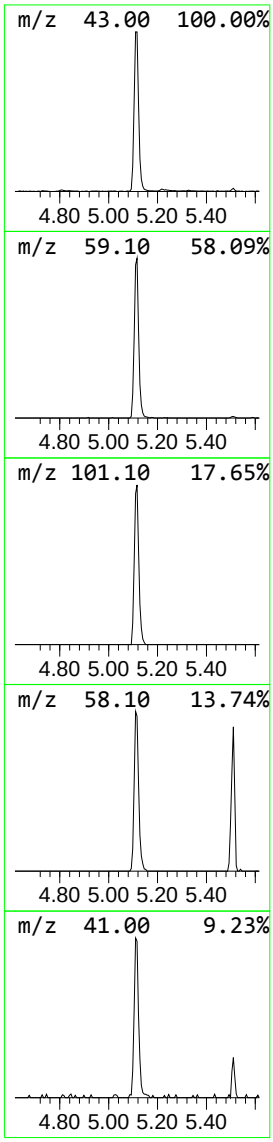
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	15.70 ng	335308	1,4-Dichlorobenzene-d4	6.886

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

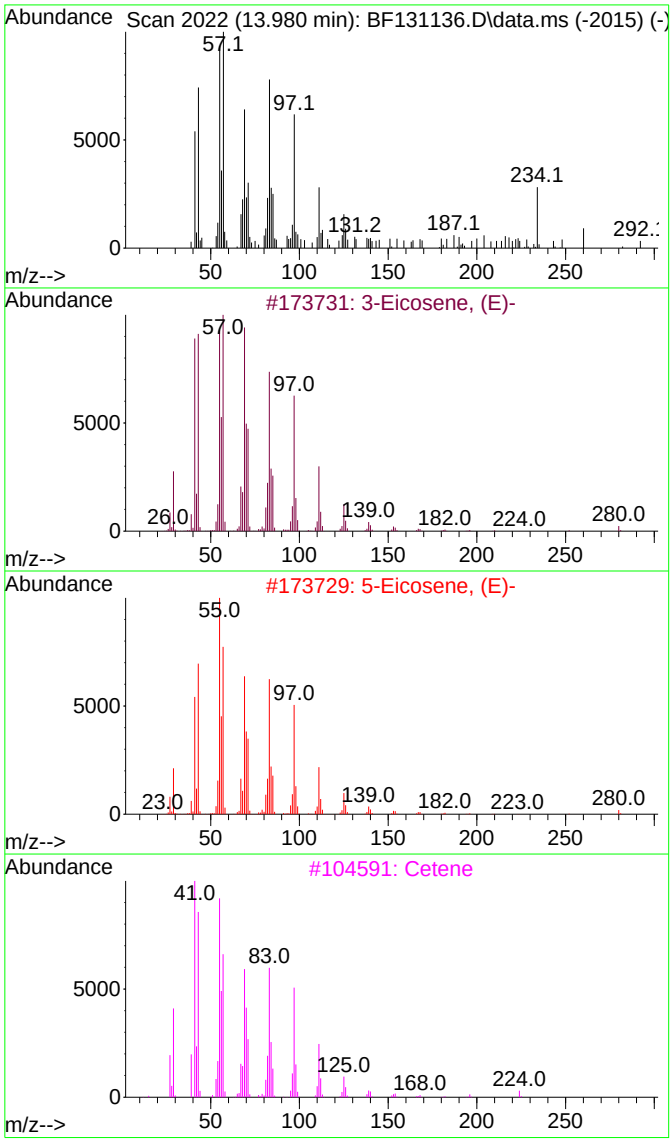
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

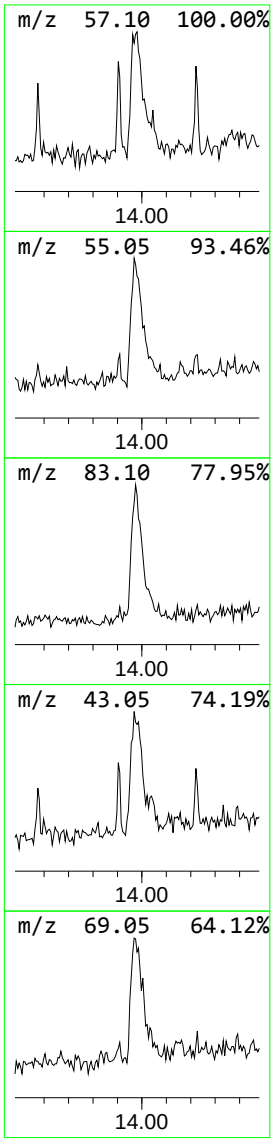
****

Peak Number 4 3-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	5.00 ng	156745	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	72
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	72
3	Cetene	224	C16H32	000629-73-2	68
4	17-Pentatriacontene	491	C35H70	006971-40-0	64
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

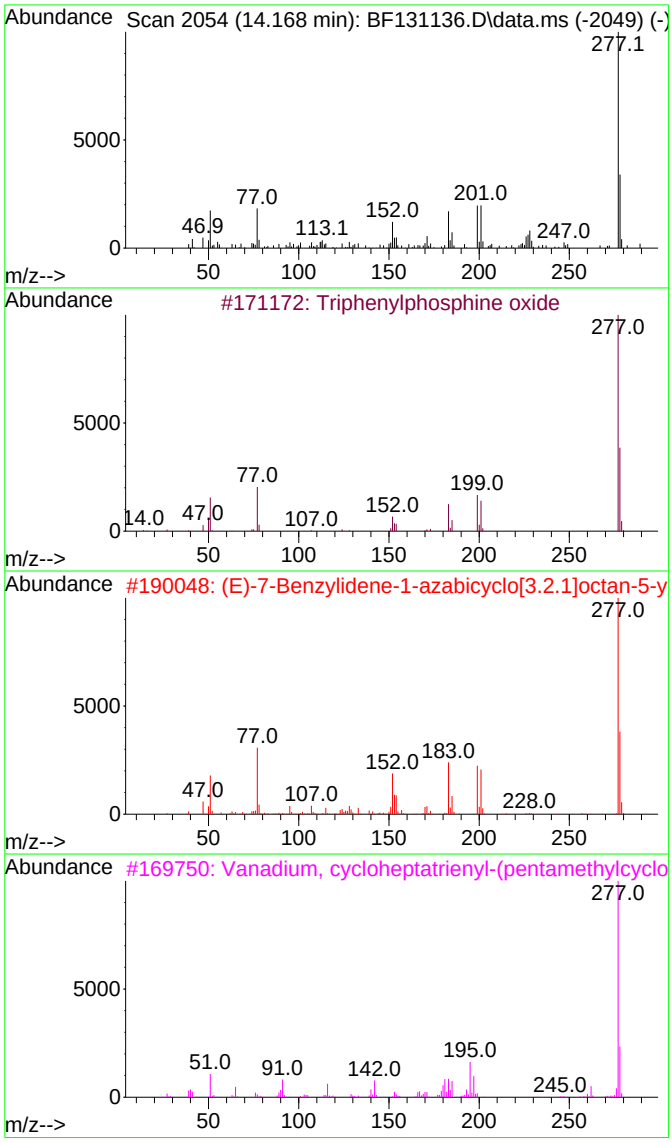
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

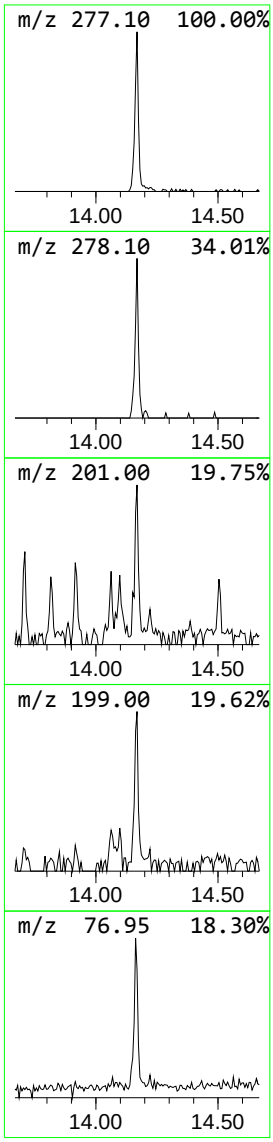
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.168	2.99 ng	93815	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	86
3	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	52
4	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	47
5	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

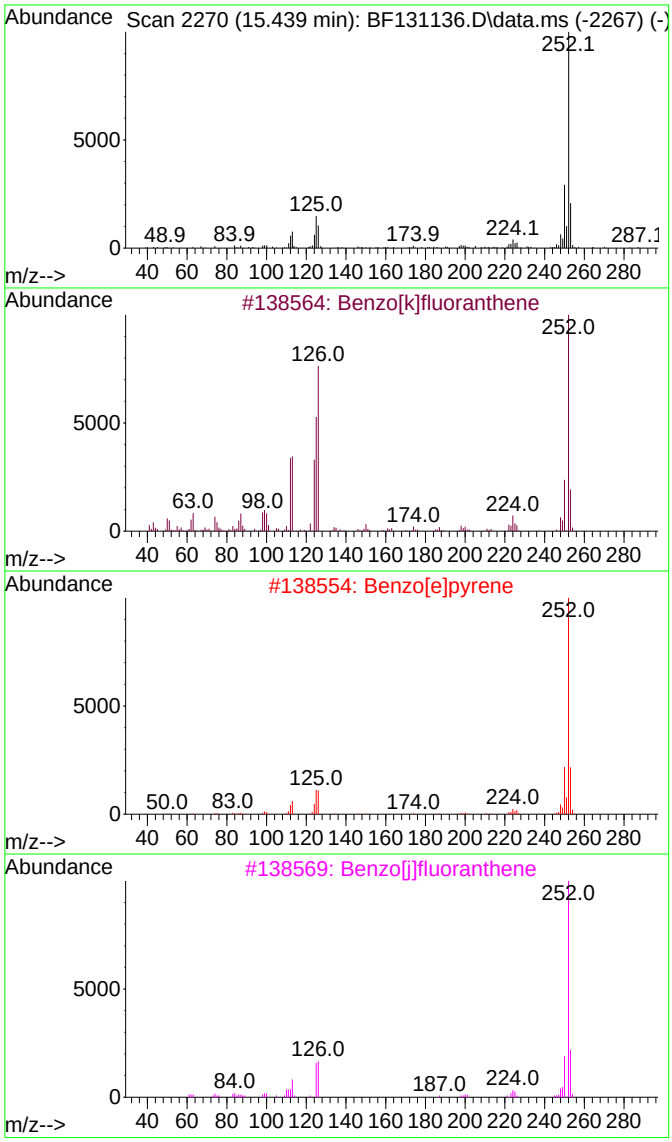
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

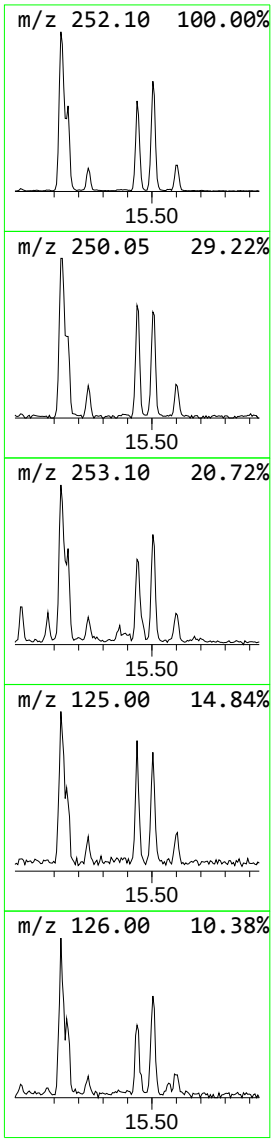
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.439	6.32 ng	129170	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2	Benzo[e]pyrene	252	C20H12	000192-97-2	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	90
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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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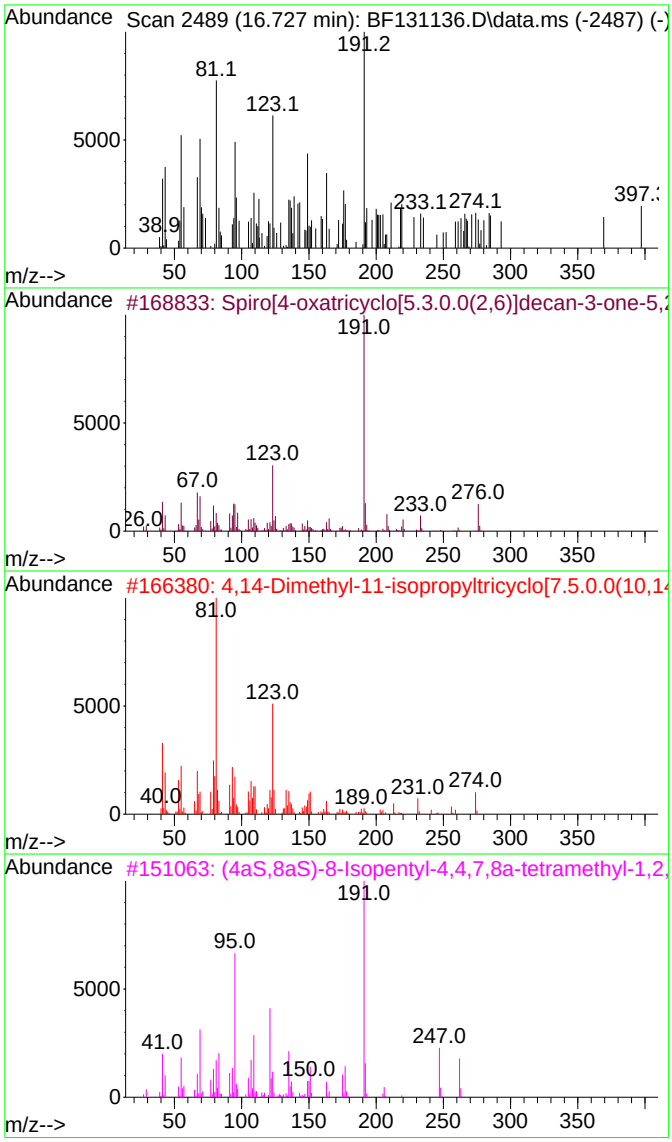
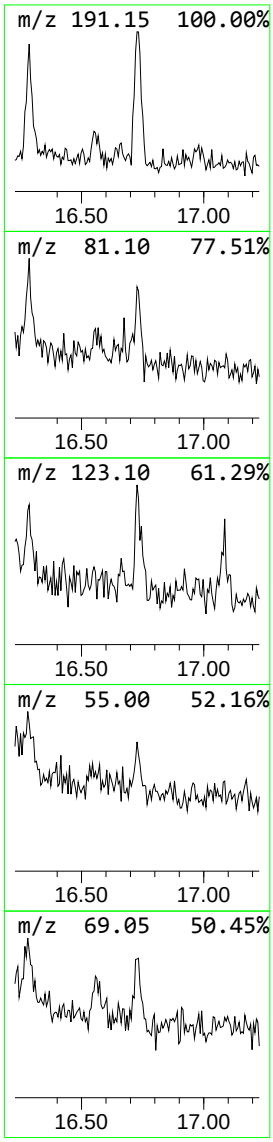
Peak Number 7 unknown16.727 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.727	2.68 ng	54705	Perylene-d12	15.568

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[4-oxatricyclo[5.3.0.0(2,6)...	276	C18H28O2	1000156-82-9	38
2	4,14-Dimethyl-11-isopropyltricyc...	274	C19H30O	1010140-68-0	25
3	(4aS,8aS)-8-Isopentyl-4,4,7,8a-t...	262	C19H34	220766-79-0	22
4	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	18
5	5-Amino-1,3,6-trimethyl-1,3-dihy...	191	C10H13N3O	073778-94-6	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131136.D
Acq On : 10 Nov 2022 22:12
Operator : CG\JU
Sample : N5524-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11995

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.175	32.3	ng	690713	1	6.886	427205	20.0
Propane, 1,1-di...	2.287	2.5	ng	53231	1	6.886	427205	20.0
2-Pentanone, 4-...	5.116	15.7	ng	335308	1	6.886	427205	20.0
3-Eicosene, (E)-	13.980	5.0	ng	156745	5	14.074	627294	20.0
Triphenylphosph...	14.168	3.0	ng	93815	5	14.074	627294	20.0
Benzo[e]pyrene	15.439	6.3	ng	129170	6	15.568	408496	20.0
unknown16.727	16.727	2.7	ng	54705	6	15.568	408496	20.0