LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

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:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.551	500	504	527	rBV	58638	203327	8.51%	0.993%
2	5.234	615	620	649	rBV	1109550	2043113	85.47%	9.981%
3	6.910	900	905	915	rBV	1266729	1924892	80.52%	9.404%
4	6.992	915	919	935	rVB	1450789	2333043	97.59%	11.398%
5	7.334	973	977	989	rBV	310634	400954	16.77%	1.959%
6	7.575	1012	1018	1031	rBV	1226748	1668999	69.82%	8.154%
7	8.257	1129	1134	1151	rBV	878484	1257557	52.61%	6.144%
8	9.363	1318	1322	1343	rBV	366510	546434	22.86%	2.670%
9	11.145	1619	1625	1638	rBV	1809130	2390546	100.00%	11.679%
10	11.839	1739	1743	1755	rVB	195290	244897	10.24%	1.196%
11	12.186	1797	1802	1808	rBV2	447851	570693	23.87%	2.788%
12	13.045	1942	1948	1953	rBB	21708	29319	1.23%	0.143%
13	13.480	2017	2022	2039	rBV	783463	1088112	45.52%	5.316%
14	13.810	2073	2078	2088	rBV	26613	48063	2.01%	0.235%
15	14.580	2205	2209	2214	rBV	341450	474740	19.86%	2.319%
16	15.545	2366	2373	2378	rBV2	14388	27553	1.15%	0.135%
17	15.604	2378	2383	2396	rVB3	89605	124178	5.19%	0.607%
18	16.398	2513	2518	2524	rBV	162073	204426	8.55%	0.999%
19	16.704	2565	2570	2578	rBV	216690	281557	11.78%	1.375%
20	16.957	2607	2613	2617	rBV	1455129	1689338	70.67%	8.253%
21	17.315	2670	2674	2679	rBV3	21240	37352	1.56%	0.182%
22	18.209	2821	2826	2835	rVV2	84769	137868	5.77%	0.674%
23	18.298	2835	2841	2845	rVV2	437039	611323	25.57%	2.987%
24	18.333	2845	2847	2851	rVV	97446	127414	5.33%	0.622%
25	18.368	2851	2853	2858	rVV2	29719	38262	1.60%	0.187%
26	18.427	2859	2863	2868	rVB2	26058	33676	1.41%	0.165%
27	18.809	2924	2928	2933	rVB	21963	26159	1.09%	0.128%
28	19.439	3028	3035	3038	rBV4	22393	43490	1.82%	0.212%
29	19.568	3053	3057	3060	rVV	180146	246482	10.31%	1.204%
30	19.598	3060	3062	3069	rVV2	65007	92399	3.87%	0.451%
31	19.686	3073	3077	3080	rVV	27783	33911	1.42%	0.166%
32	19.803	3094	3097	3102	rVB7	14020	24238	1.01%	0.118%
33	19.856	3102	3106	3112	rBV	107036	118242	4.95%	0.578%
34	19.915	3112	3116	3121	rBV	156079	176536	7.38%	0.862%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

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:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.968	3121	3125	3134	rVV	292079	383685	16.05%	1.874%
36	20.074	3140	3143	3149	rVB7	20160	33149	1.39%	0.162%
37	20.445	3202	3206	3209	rVV4	24037	37823	1.58%	0.185%
38	20.480	3209	3212	3216	rVB3	38362	44173	1.85%	0.216%
39	20.797	3258	3266	3273	rVB6	39991	92556	3.87%	0.452%
40	20.980	3292	3297	3301	rBV5	20132	37299	1.56%	0.182%
41	21.144	3318	3325	3331	rBV2	71695	129457	5.42%	0.632%
42	21.197	3331	3334	3342	rVB8	19042	46684	1.95%	0.228%
43	21.274	3342	3347	3351	rBV2	25356	44117	1.85%	0.216%
44	21.474	3376	3381	3390	rVB	57620	118802	4.97%	0.580%
45	21.686	3413	3417	3422	rVB6	16826	31348	1.31%	0.153%
46	23.168	3664	3669	3677	rVB2	12374	34984	1.46%	0.171%
47	24.033	3802	3816	3827	rBV10	29107	136323	5.70%	0.666%

Sum of corrected areas: 20469493

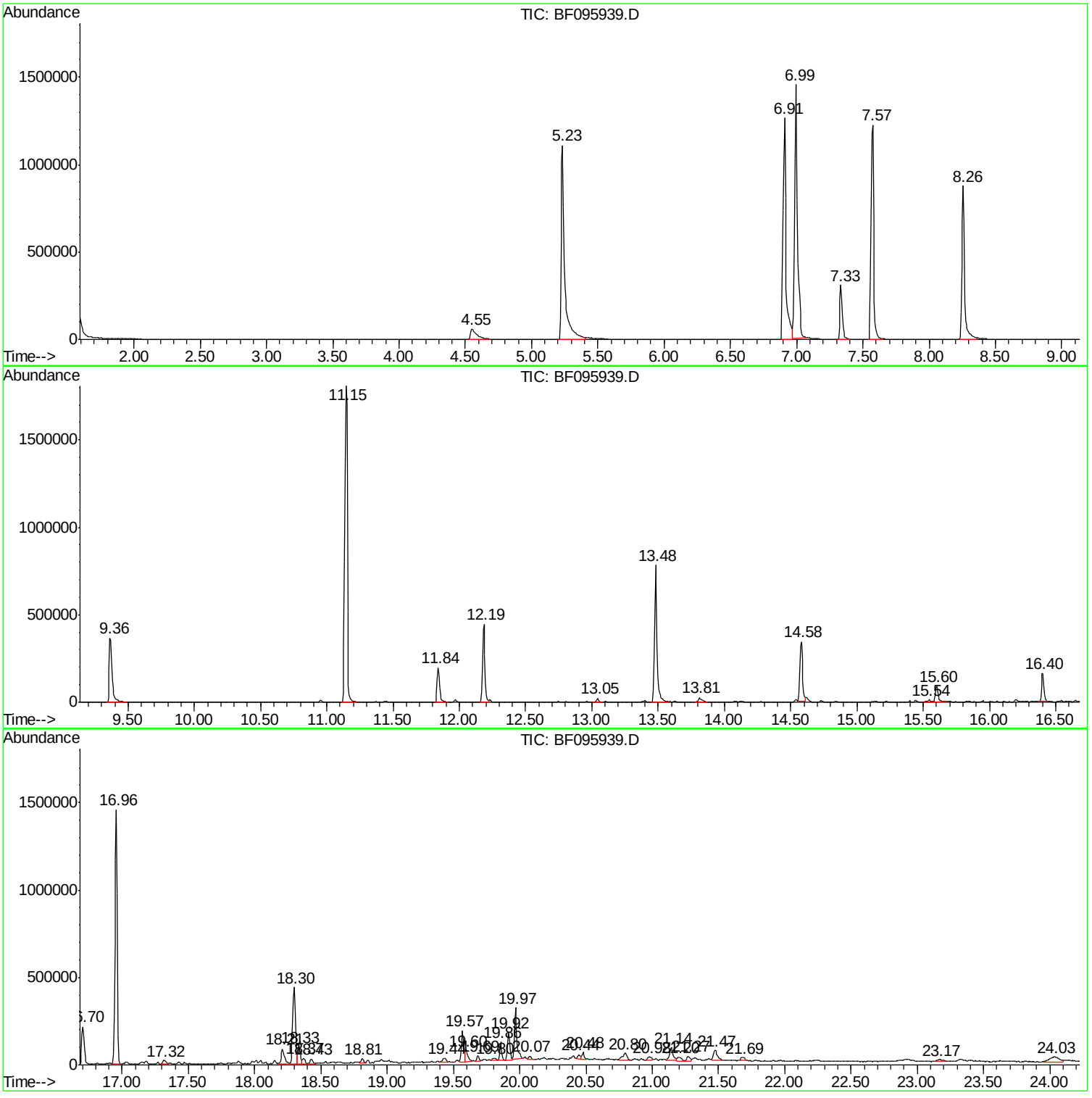
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

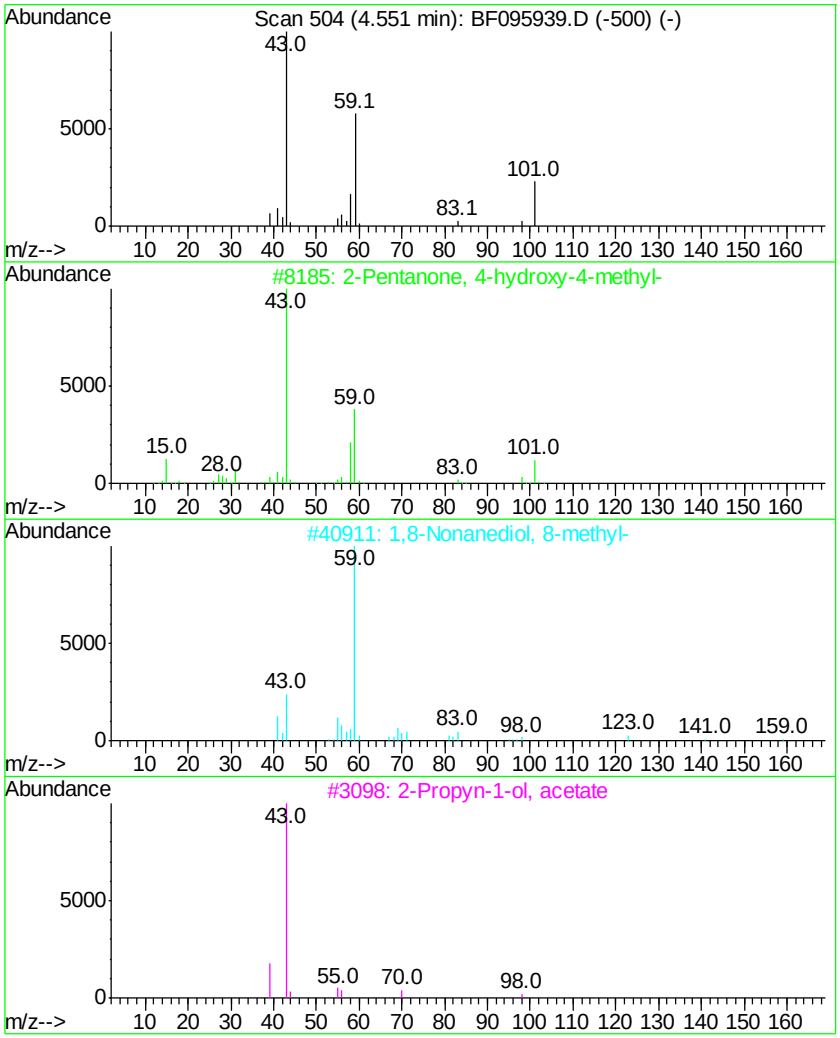
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

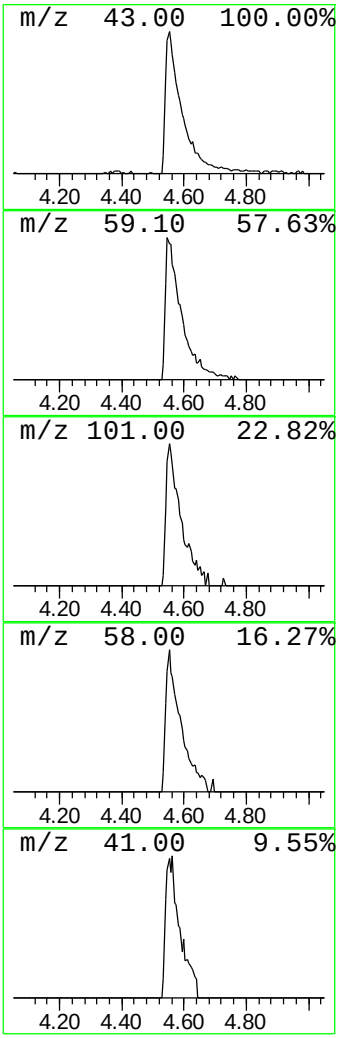
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	10.14 ng	203327	1,4-Dichlorobenzene-d4	7.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

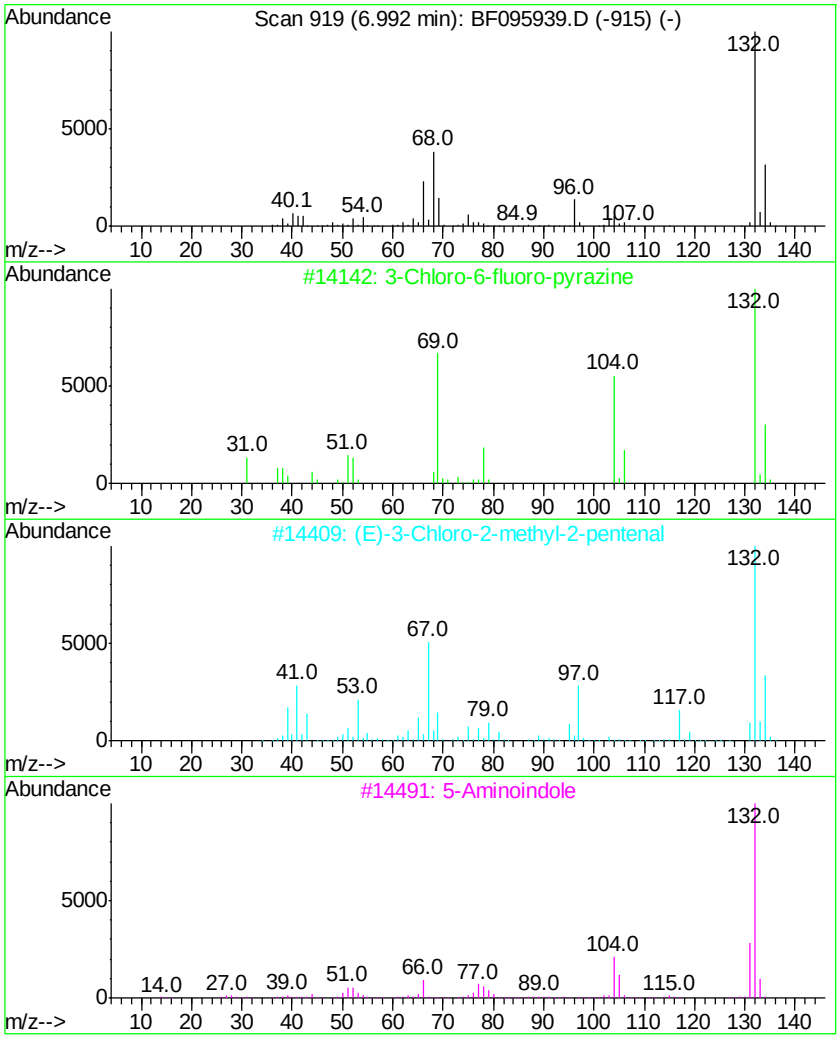
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

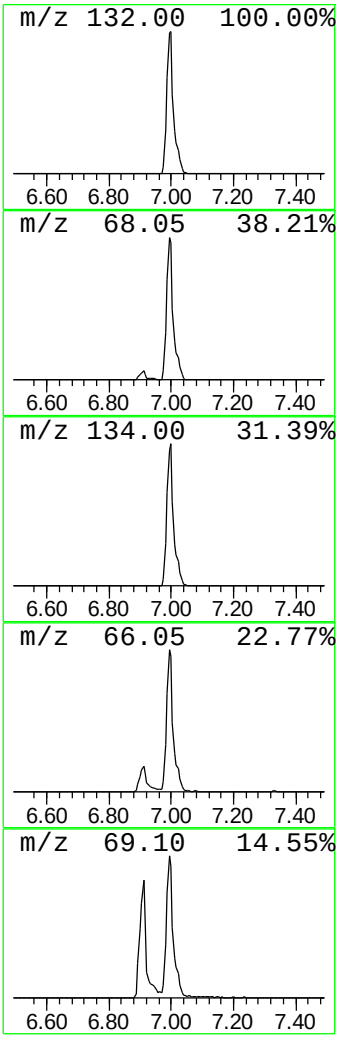
****

Peak Number 2 unknown6.99 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	116.38 ng	2333040	1,4-Dichlorobenzene-d4	7.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

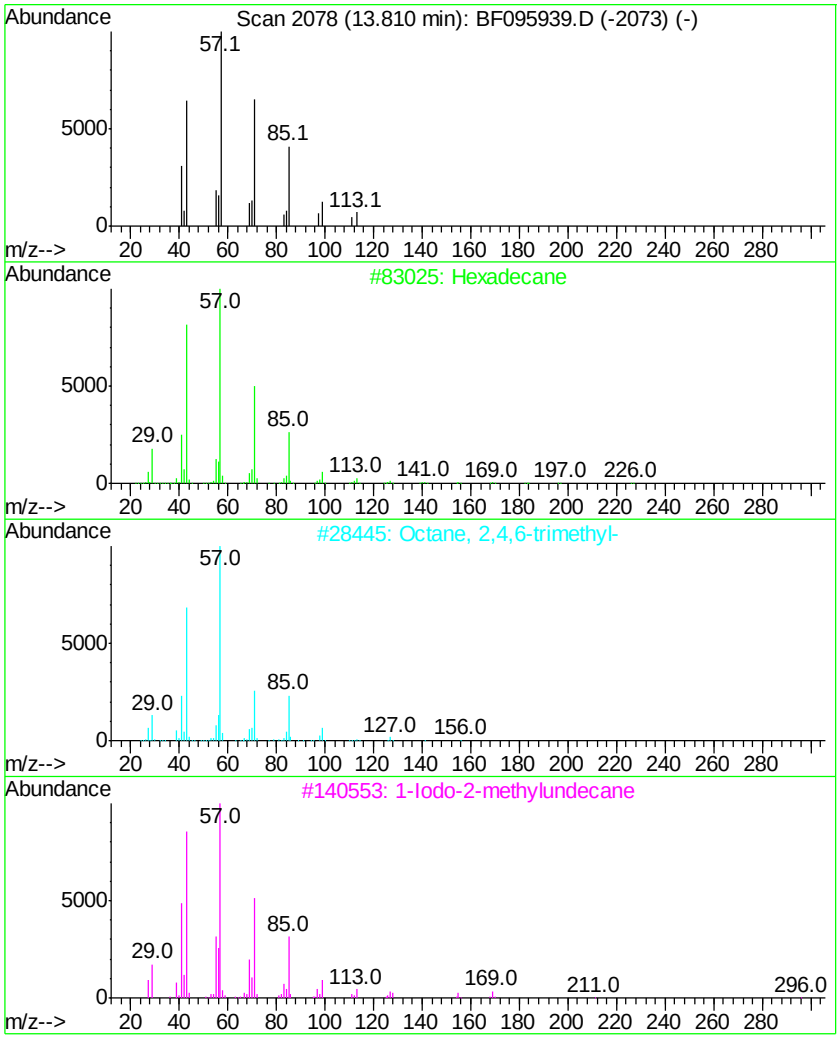
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

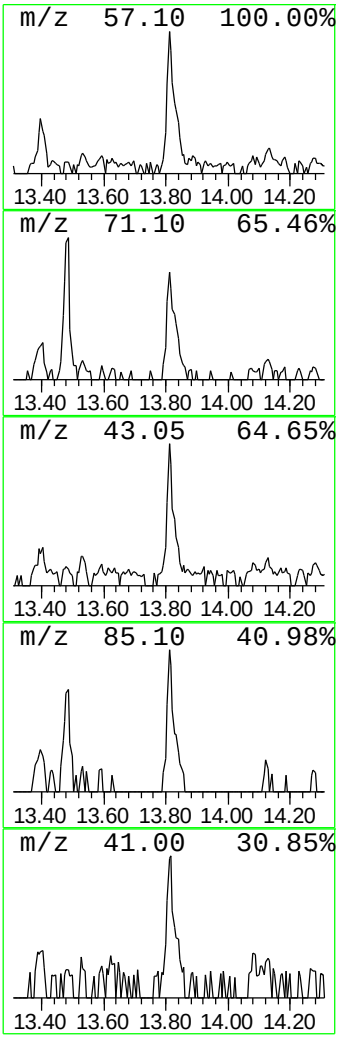
****

Peak Number 4 Hexadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.02 ng	48063	Phenanthrene-d10	14.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	78
3	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	78
4	Tetradecane	198	C14H30	000629-59-4	72
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

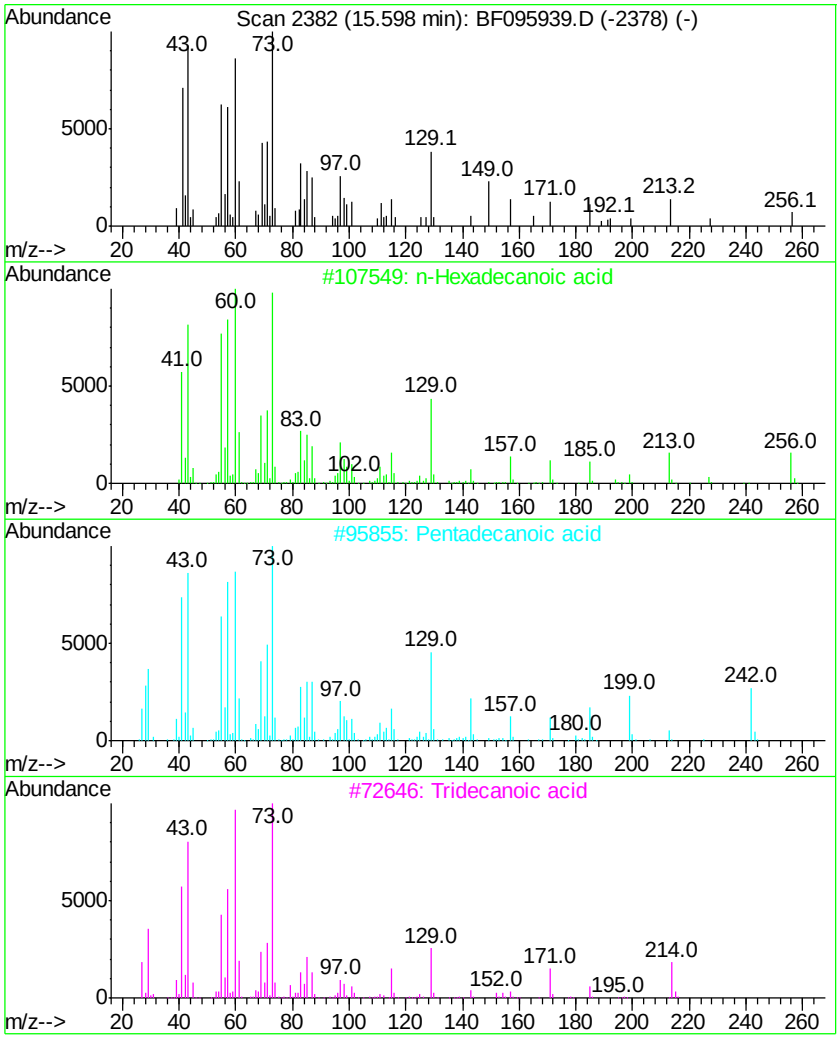
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

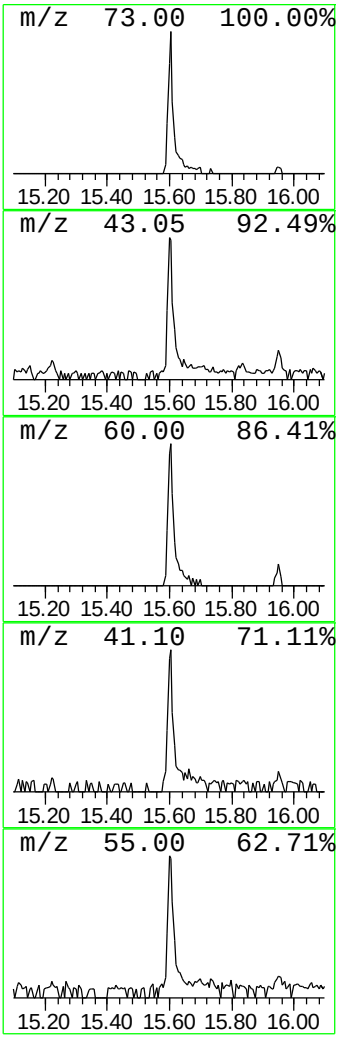
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	5.23 ng	124178	Phenanthrene-d10	14.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

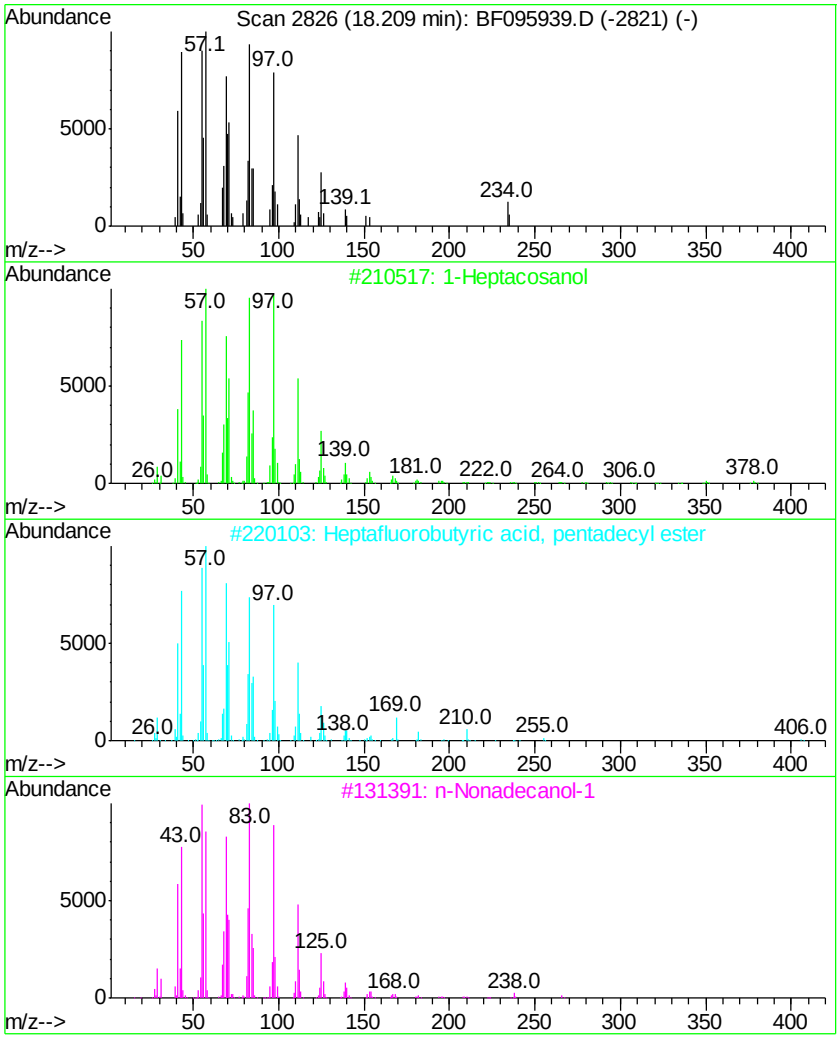
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

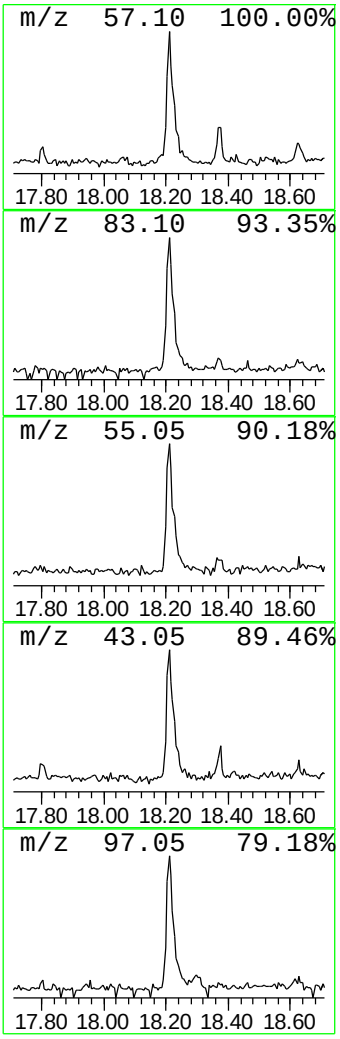
****

Peak Number 6 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	4.51 ng	137868	Chrysene-d12	18.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Octacosanol	410	C28H58O	000557-61-9	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

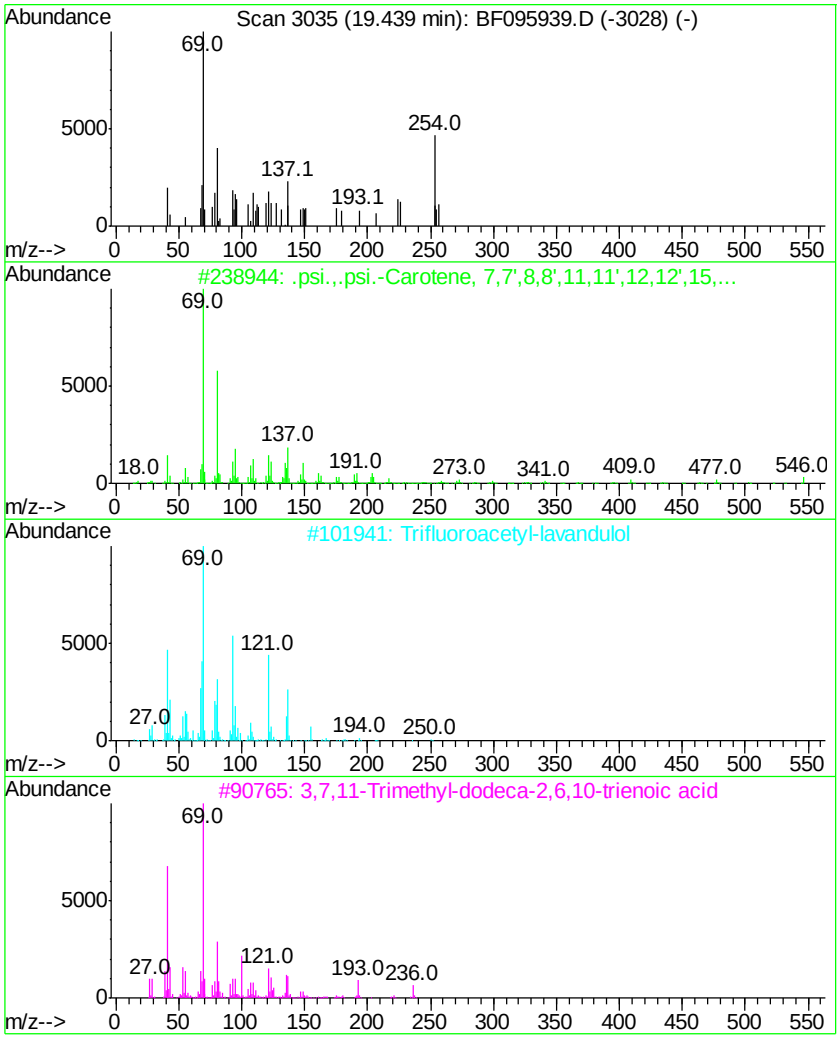
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

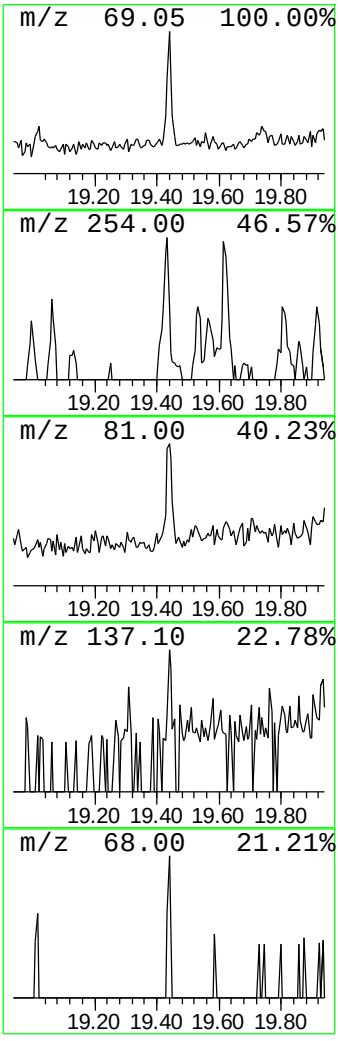
****

Peak Number 7 unknown19.44 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.44	2.27 ng	43490	Perylene-d12	19.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	38
2	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	35
3	3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	35
4	Squalene	410	C30H50	007683-64-9	32
5	Octane, 1,2-dibromo-	270	C8H16Br2	006269-92-7	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

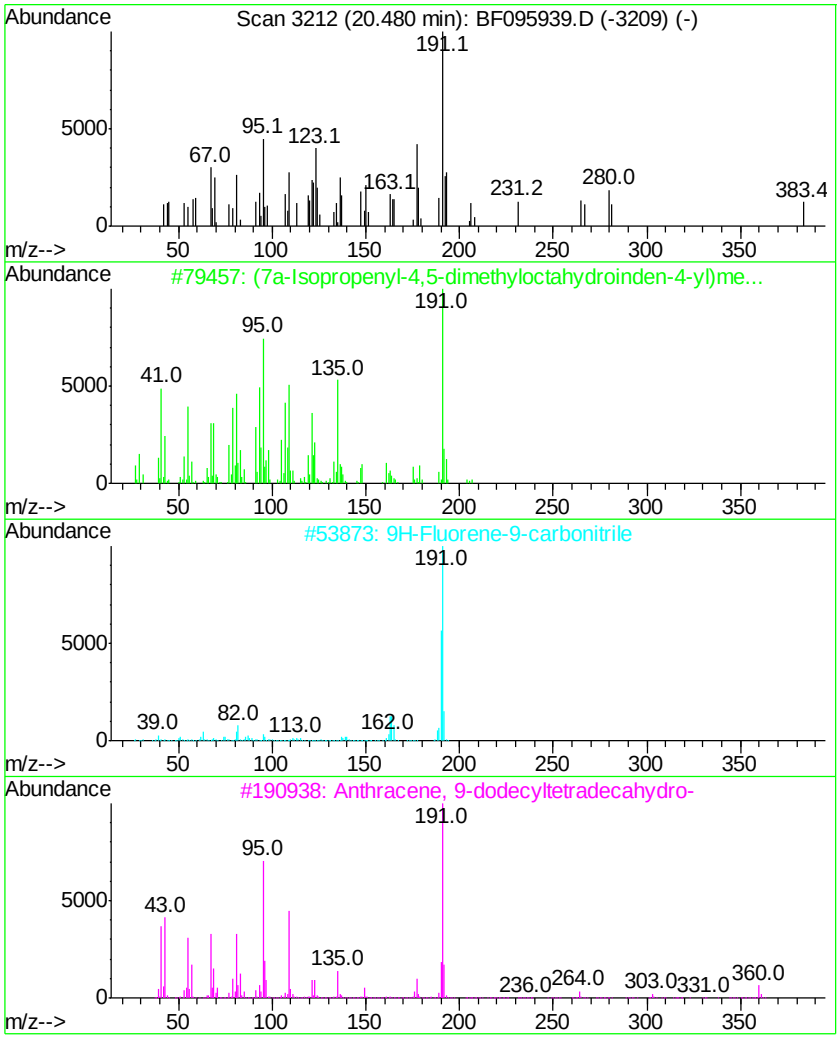
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

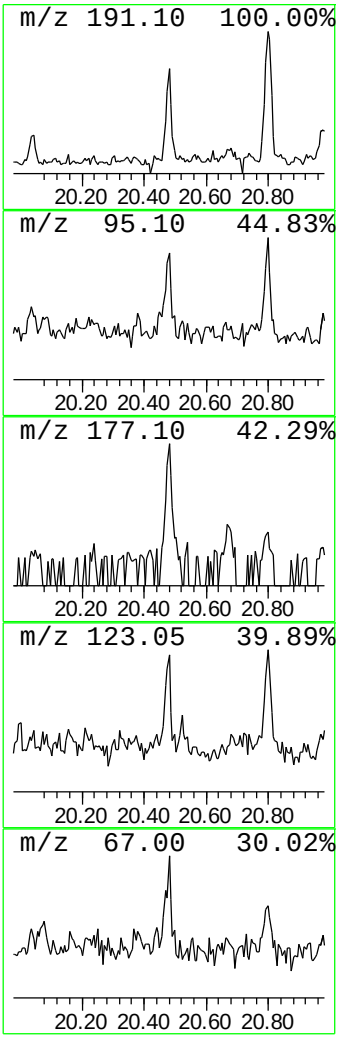
****

Peak Number 9 unknown20.48 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.48	2.30 ng	44173	Perylene-d12	19.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(7a-Isopropenyl-4,5-dimethyloctа...	222	C15H26O	1000187-02-9	38
2	9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	35
3	Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	32
4	Anthracene, 9-[2,2-bis(hydroxyme...	280	C19H20O2	144000-85-1	30
5	2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

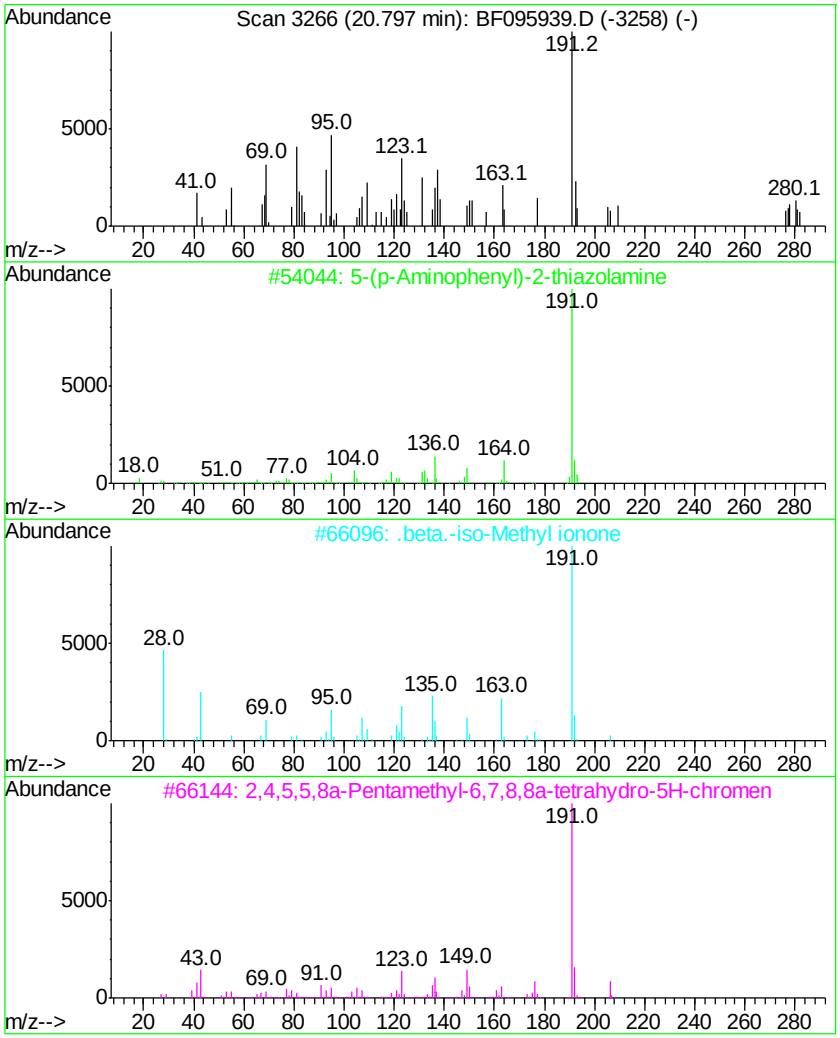
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

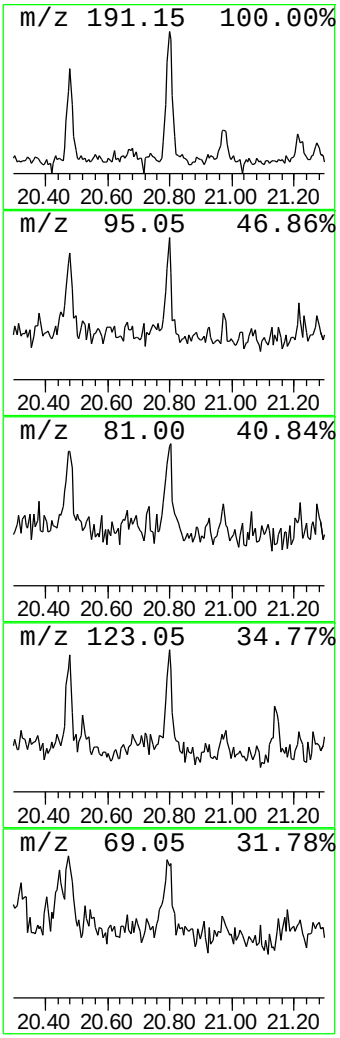
****

Peak Number 10 unknown20.80 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.80	4.82 ng	92556	Perylene-d12	19.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	43
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
3	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	37
4	(7a-Isopropenyl-4,5-dimethylocta...	222	C15H26O	1000187-02-9	37
5	N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

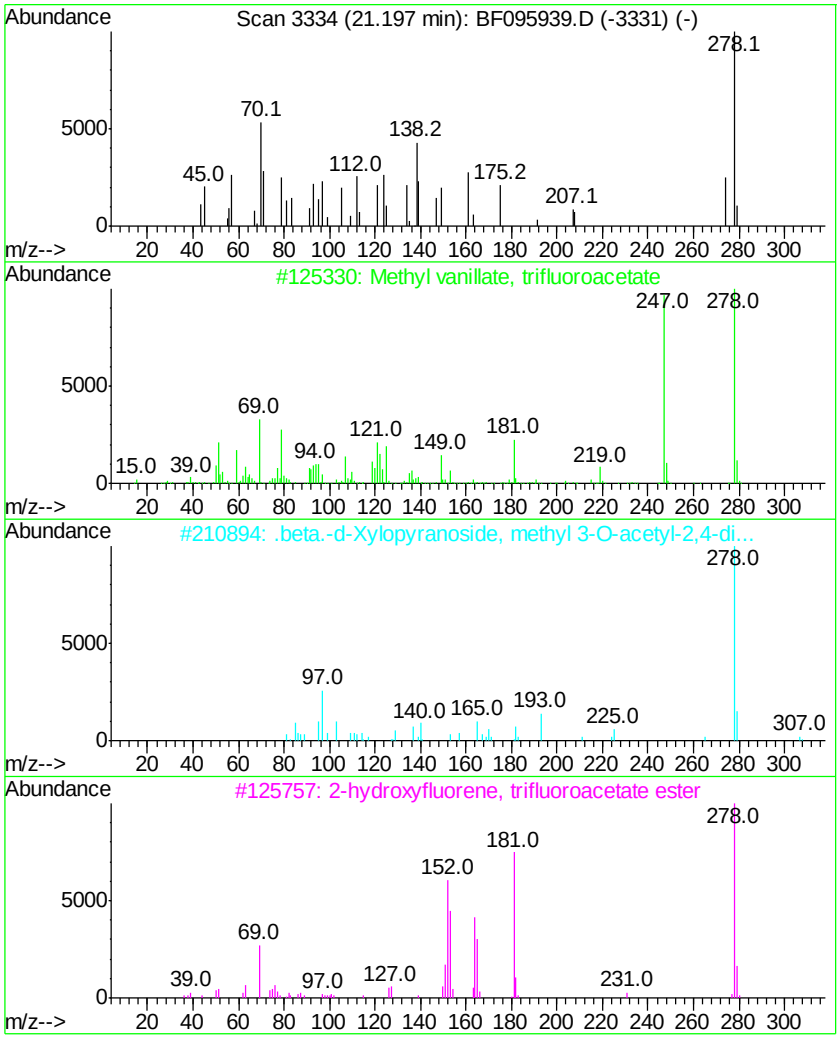
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

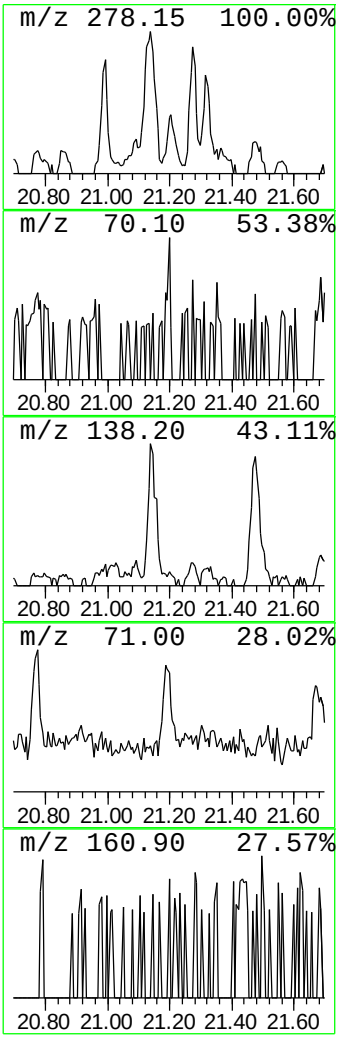
****

Peak Number 11 unknown21.20 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.20	2.43 ng	46684	Perylene-d12	19.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl vanillate, trifluoroacetate	278	C11H9F3O5	1000365-24-7	16
2	.beta.-d-Xylopyranoside, methyl ...	398	C12H12F6O8	126590-82-7	14
3	2-hydroxyfluorene, trifluoroacet...	278	C15H9F3O2	1000376-46-3	9
4	1,4-Naphthoquinone, 2-acetyl-3,5...	278	C13H10O7	015254-72-5	9
5	Dibenz[a,h]anthracene	278	C22H14	000053-70-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

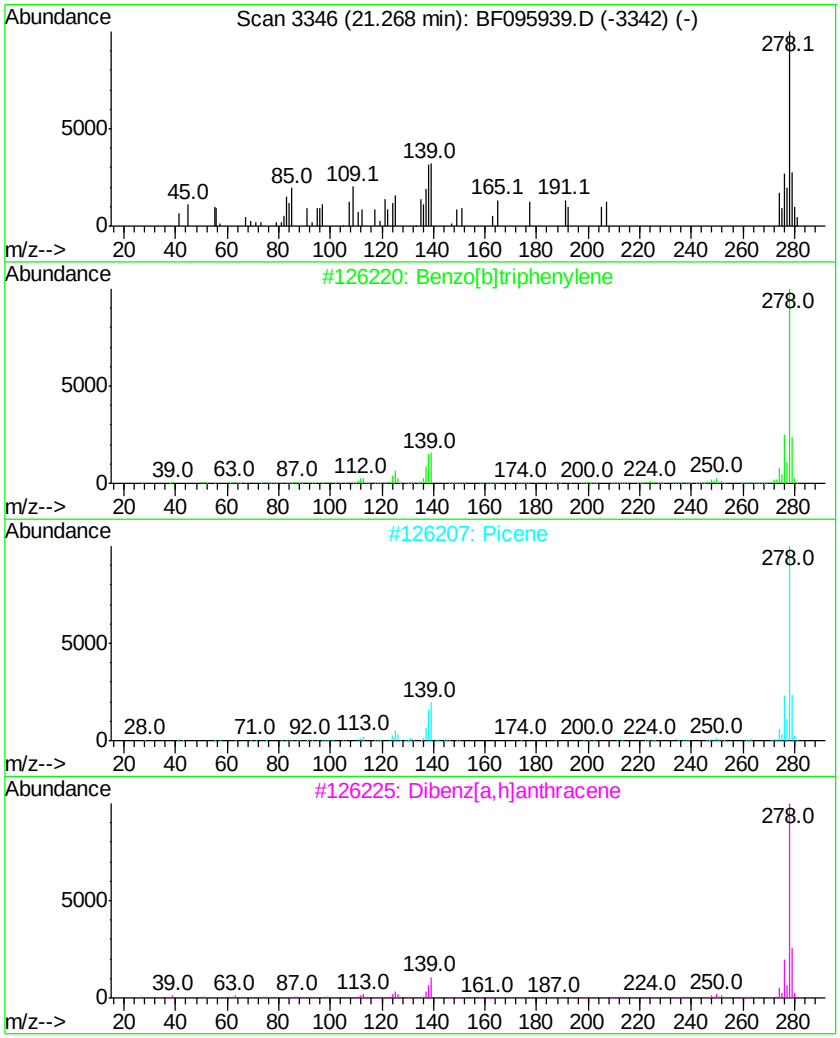
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

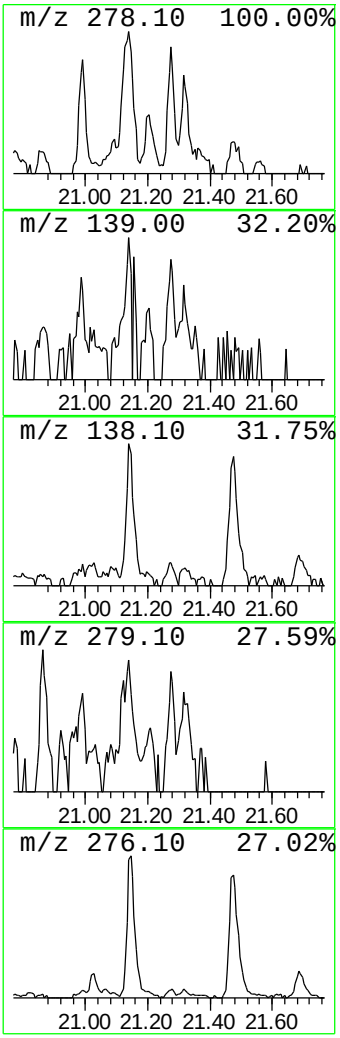
****

Peak Number 12 Benzo[b]triphenylene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	2.30 ng	44117	Perylene-d12	19.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]triphenylene	278	C22H14	000215-58-7	81
2	Picene	278	C22H14	000213-46-7	74
3	Dibenz[a,h]anthracene	278	C22H14	000053-70-3	68
4	Pentacene	278	C22H14	000135-48-8	59
5	Pyridine-3-carbonitrile, 2-oxo-4...	278	C16H10N2OS	1000304-72-3	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

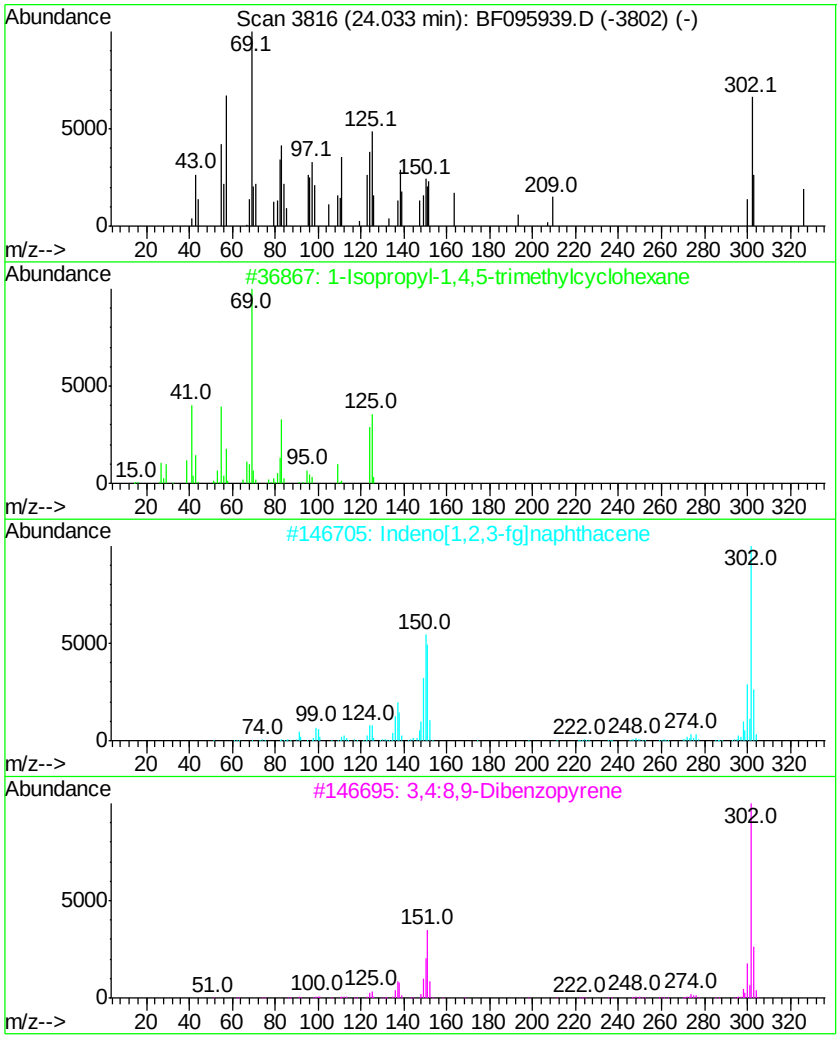
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

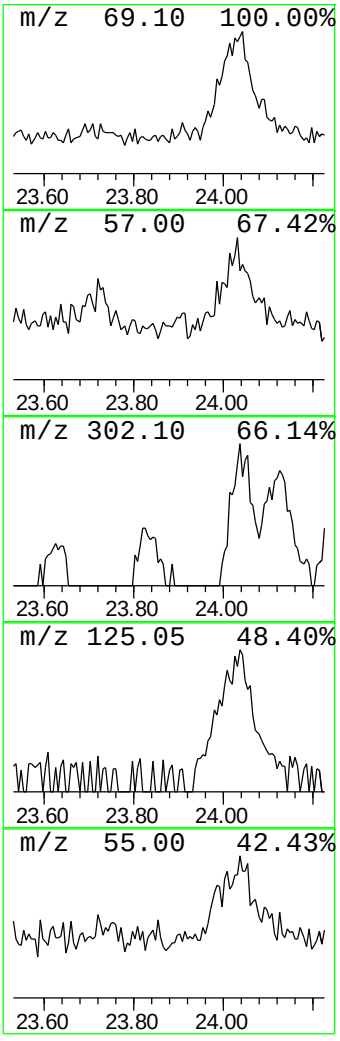
****

Peak Number 13 unknown24.03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.03	7.11 ng	136323	Perylene-d12	19.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isopropyl-1,4,5-trimethylcyclo...	168	C12H24	219783-06-9	35
2	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	22
3	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	16
4	1,3-Diisopropyl cyclohexane	168	C12H24	007045-70-7	16
5	n-Nonenylsuccinic anhydride	224	C13H20O3	028928-97-4	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061417\
Data File : BF095939.D
Acq On : 15 Jun 2017 00:05
Operator : SJ/MA
Sample : I3660-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-72-11941

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.55	10.1	ng	203327	1	7.33	400954	20.0
unknown6.99	6.99	116.4	ng	2333040	1	7.33	400954	20.0
Hexadecane	13.81	2.0	ng	48063	4	14.58	474740	20.0
n-Hexadecanoic acid	15.60	5.2	ng	124178	4	14.58	474740	20.0
1-Heptacosanol	18.21	4.5	ng	137868	5	18.30	611323	20.0
unknown19.44	19.44	2.3	ng	43490	6	19.97	383685	20.0
unknown20.48	20.48	2.3	ng	44173	6	19.97	383685	20.0
unknown20.80	20.80	4.8	ng	92556	6	19.97	383685	20.0
unknown21.20	21.20	2.4	ng	46684	6	19.97	383685	20.0
Benzo[b]triphenylene	21.27	2.3	ng	44117	6	19.97	383685	20.0
unknown24.03	24.03	7.1	ng	136323	6	19.97	383685	20.0