LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092147.D
Acq On : 9 Jan 2017 19:42
Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

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-BF122116.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	2.058	14	15	24	rVB4	17774	54951	1.04%	0.114%
2	4.767	249	252	260	rBV	1554068	2427910	45.75%	5.041%
3	5.236	291	293	296	rBV	4659192	5307357	100.00%	11.021%
4	6.299	383	386	389	rBV	3389661	4762713	89.74%	9.890%
5	6.402	393	395	398	rVV	3335033	4733049	89.18%	9.828%
6	6.459	398	400	408	rVB2	23455	66455	1.25%	0.138%
7	6.630	413	415	417	rBV	1147139	990641	18.67%	2.057%
8	6.790	426	429	431	rBV	3692380	3866617	72.85%	8.029%
9	7.202	462	465	467	rBV	2799095	2800765	52.77%	5.816%
10	7.339	474	477	482	rVB	74929	92436	1.74%	0.192%
11	7.922	525	528	531	rBV	1180056	1468340	27.67%	3.049%
12	8.630	588	590	592	rBV	92182	78135	1.47%	0.162%
13	8.733	596	599	601	rVB	60589	71803	1.35%	0.149%
14	8.996	619	622	625	rBV	4061113	4684757	88.27%	9.728%
15	9.099	627	631	632	rVB3	42593	61653	1.16%	0.128%
16	9.396	655	657	660	rBV	1317521	1198433	22.58%	2.489%
17	9.533	667	669	671	rVB	72670	100671	1.90%	0.209%
18	9.670	678	681	682	rBV	1292855	1316827	24.81%	2.734%
19	9.693	682	683	686	rVB	45416	55428	1.04%	0.115%
20	10.093	714	718	719	rBV2	34332	68959	1.30%	0.143%
21	10.208	727	728	732	rBV	47342	57827	1.09%	0.120%
22	10.459	747	750	752	rBV	2762051	2796236	52.69%	5.806%
23	10.573	757	760	766	rVV2	204297	293371	5.53%	0.609%
24	11.031	798	800	802	rBV2	81998	72381	1.36%	0.150%
25	11.145	807	810	811	rBV	1294479	1176964	22.18%	2.444%
26	11.213	814	816	818	rVB	78793	101636	1.92%	0.211%
27	11.396	829	832	835	rBV	111930	186618	3.52%	0.388%
28	11.453	835	837	840	rVB2	53535	73141	1.38%	0.152%
29	11.648	849	854	855	rBV4	45161	89815	1.69%	0.186%
30	11.693	857	858	862	rVV2	358802	427567	8.06%	0.888%
31	11.751	862	863	869	rVB	92400	163602	3.08%	0.340%
32	12.208	899	903	906	rBV3	75016	156407	2.95%	0.325%
33	12.345	914	915	918	rBV	144794	207289	3.91%	0.430%
34	12.482	925	927	929	rBV2	54708	81918	1.54%	0.170%

LSC Area Percent Report

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Sample : I1064-09
Misc :
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Instrument : BNA_F
ClientSampleId : TP4-COMP12

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.574	933	935	938	rBV	361847	418285	7.88%	0.869%
36	12.734	946	949	951	rBV	3683330	3441574	64.85%	7.146%
37	12.905	961	964	966	rVB	56906	91995	1.73%	0.191%
38	12.974	968	970	972	rVV	62192	68117	1.28%	0.141%
39	13.008	972	973	977	rVB	51536	70598	1.33%	0.147%
40	13.225	989	992	994	rVB	284592	340600	6.42%	0.707%
41	13.637	1026	1028	1034	rBV2	158080	251698	4.74%	0.523%
42	13.774	1037	1040	1047	rVV2	1100178	1295825	24.42%	2.691%
43	14.539	1105	1107	1108	rBV	40921	53287	1.00%	0.111%
44	14.768	1125	1127	1131	rVB	142580	228520	4.31%	0.475%
45	15.031	1148	1150	1153	rBV	142747	173351	3.27%	0.360%
46	15.088	1153	1155	1157	rVV	187802	221920	4.18%	0.461%
47	15.145	1157	1160	1167	rVB	734599	911450	17.17%	1.893%
48	16.403	1268	1270	1274	rVB	77882	151900	2.86%	0.315%
49	16.791	1301	1304	1307	rVB	85513	167972	3.16%	0.349%
50	18.734	1469	1474	1476	rBV5	43843	178976	3.37%	0.372%

Sum of corrected areas: 48158740

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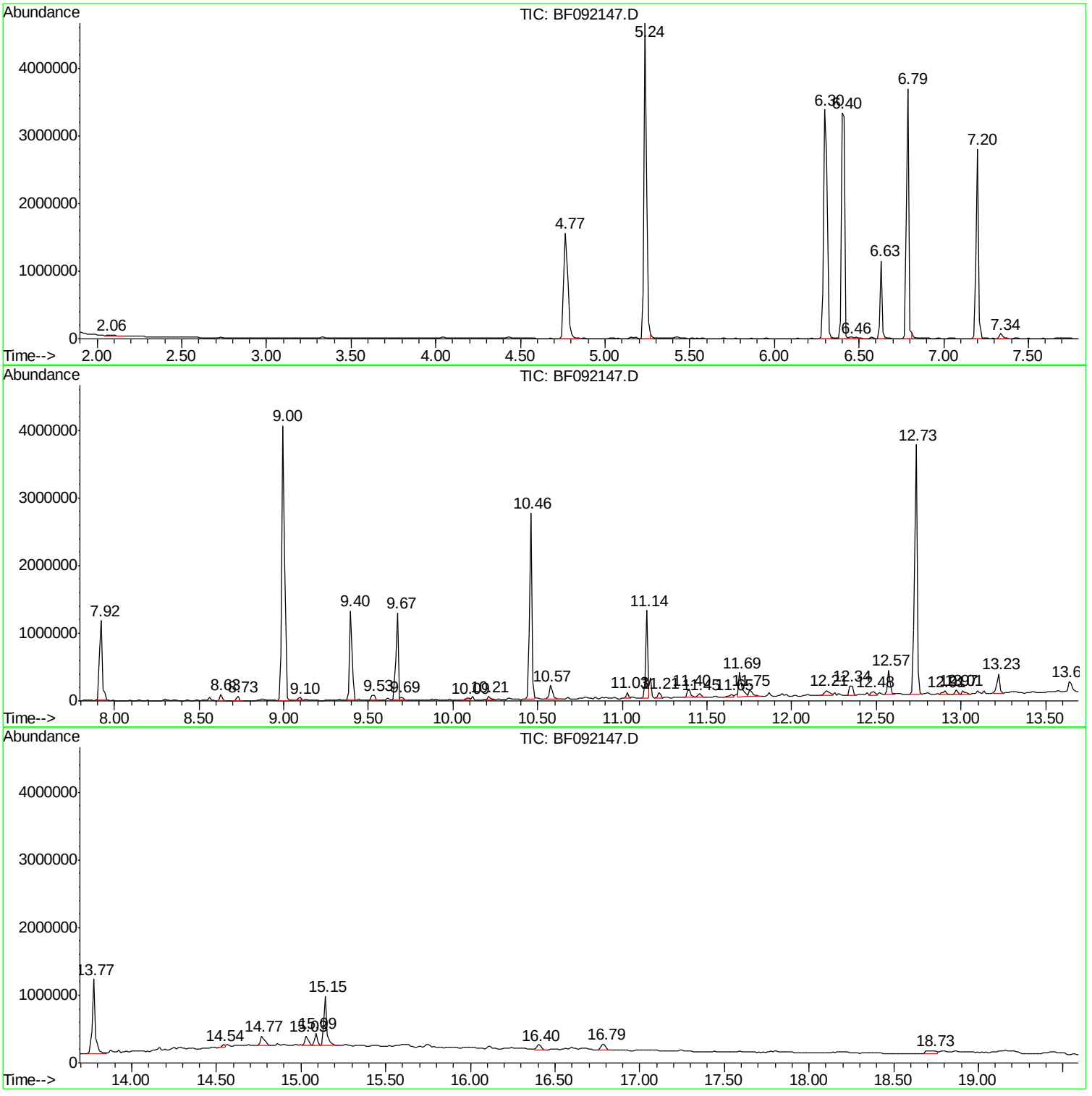
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

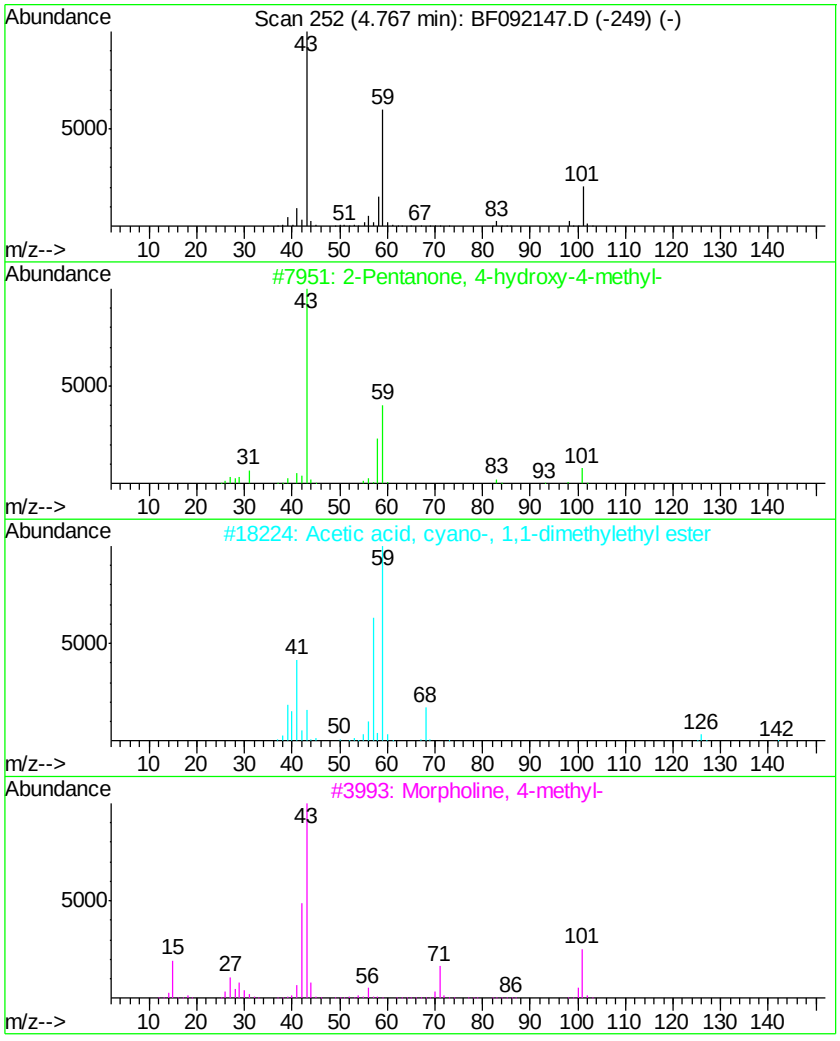
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

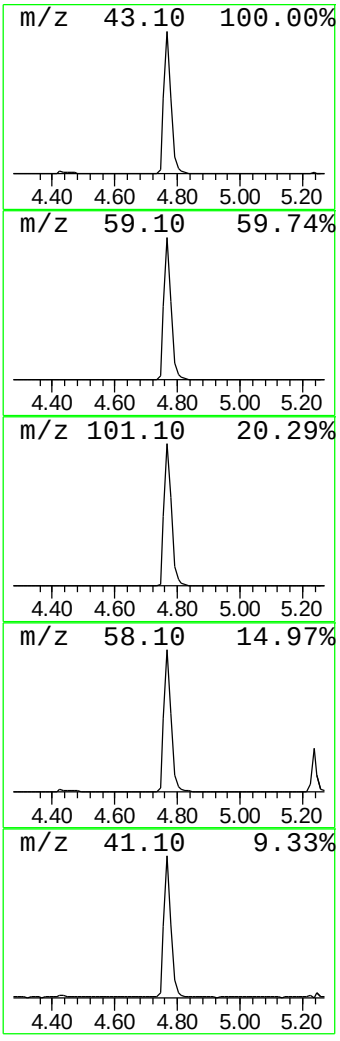
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	49.02 ng	2427910	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : I1064-09
Misc :
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Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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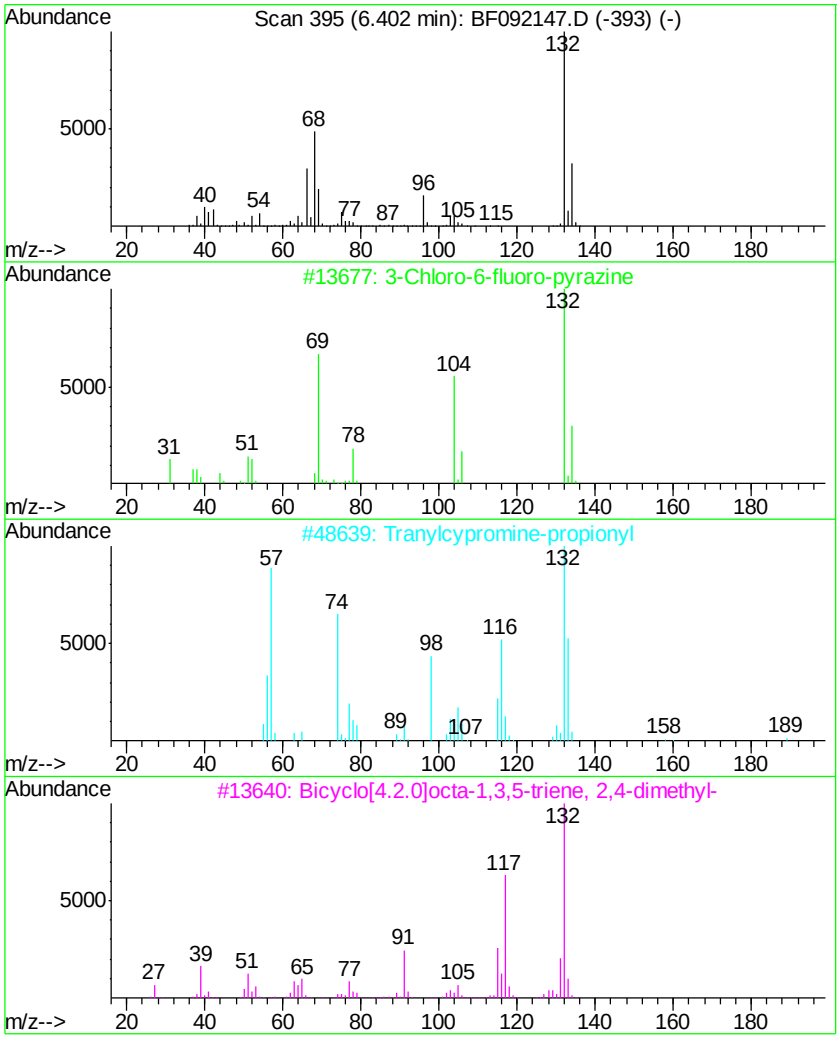
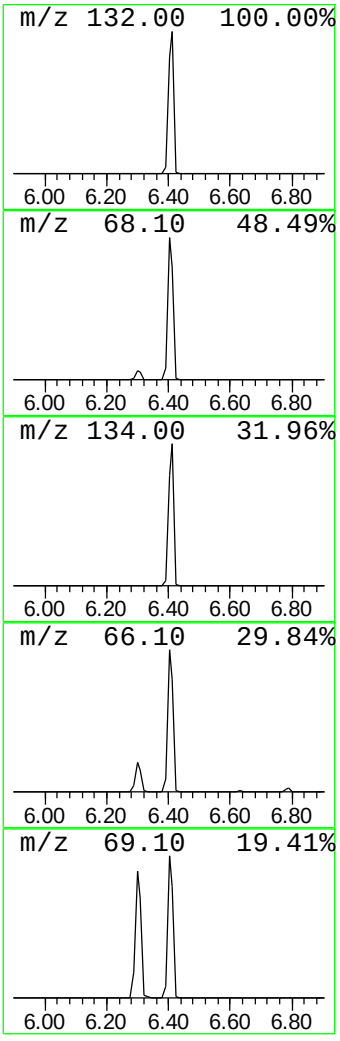
Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	95.56 ng	4733050	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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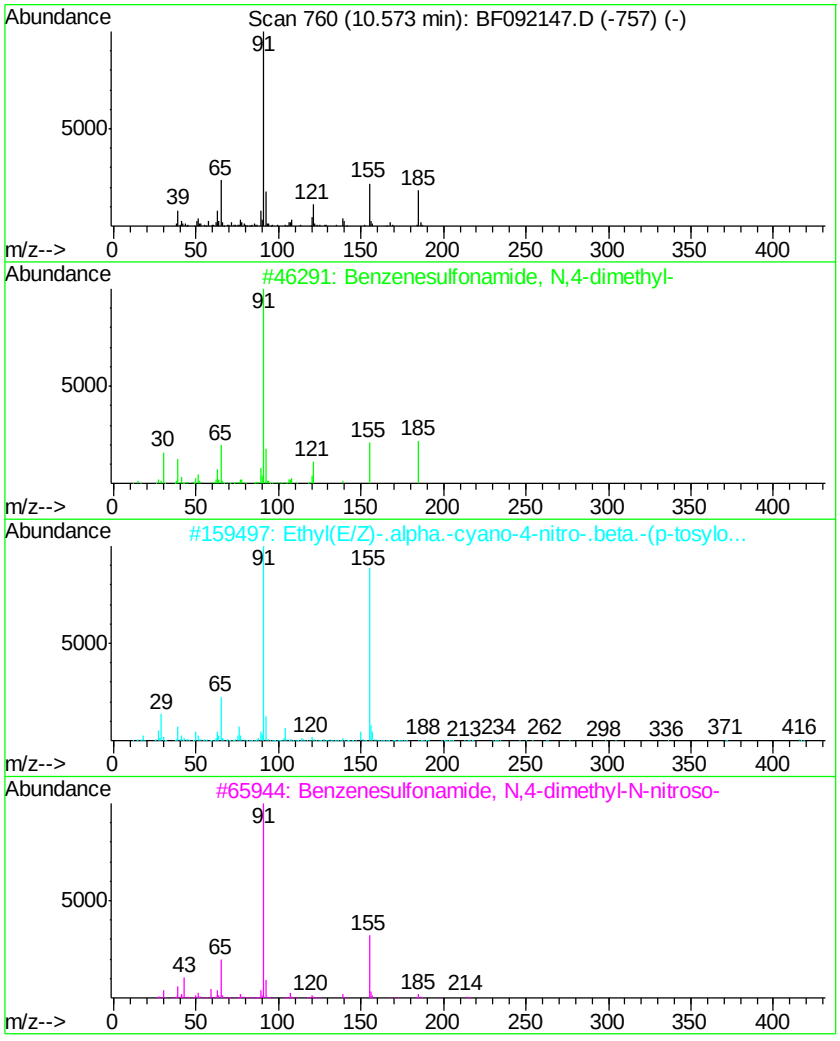
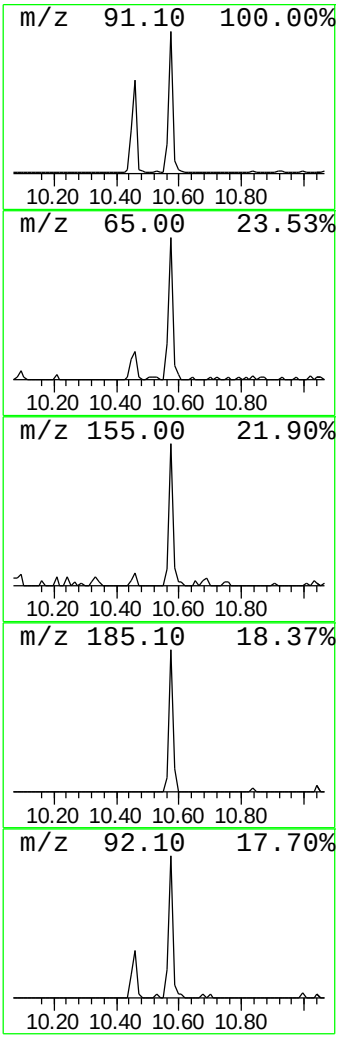
Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	4.99 ng	293371	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	93
2	Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	53
3	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	53
4	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	50
5	(O-p-Tosylisonitroso)malononitrile	249	C10H7N3O3S	020893-01-0	50





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Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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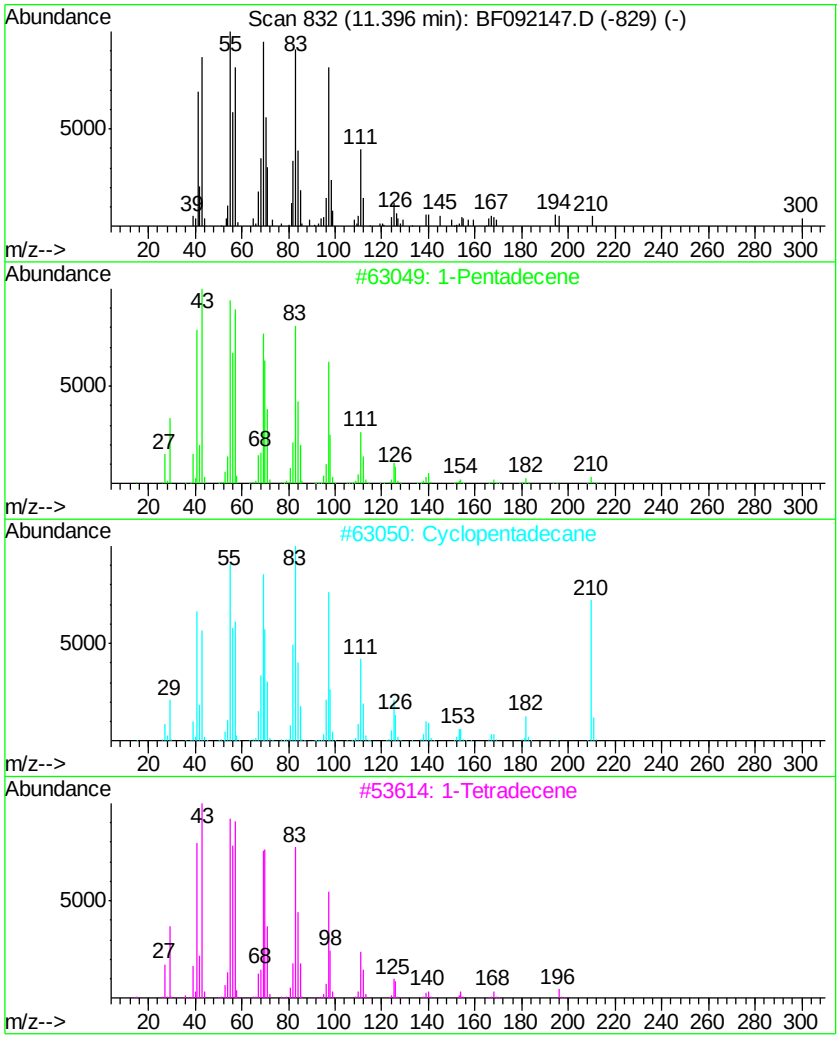
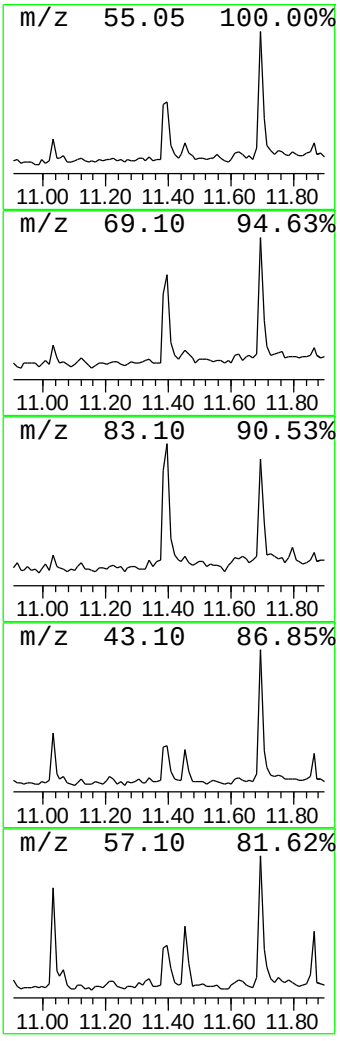
Peak Number 5 1-Pentadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	3.17 ng	186618	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene	210	C15H30	013360-61-7	97
2	Cyclopentadecane	210	C15H30	000295-48-7	96
3	1-Tetradecene	196	C14H28	001120-36-1	95
4	Cyclotetradecane	196	C14H28	000295-17-0	95
5	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	91





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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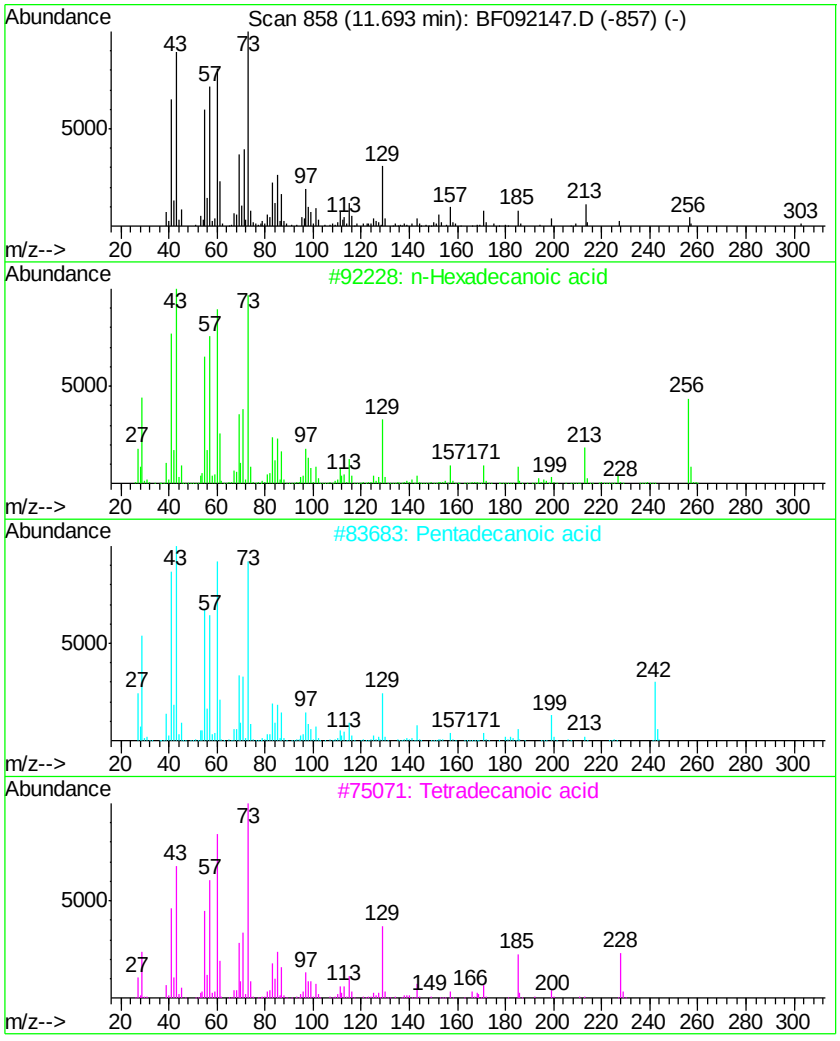
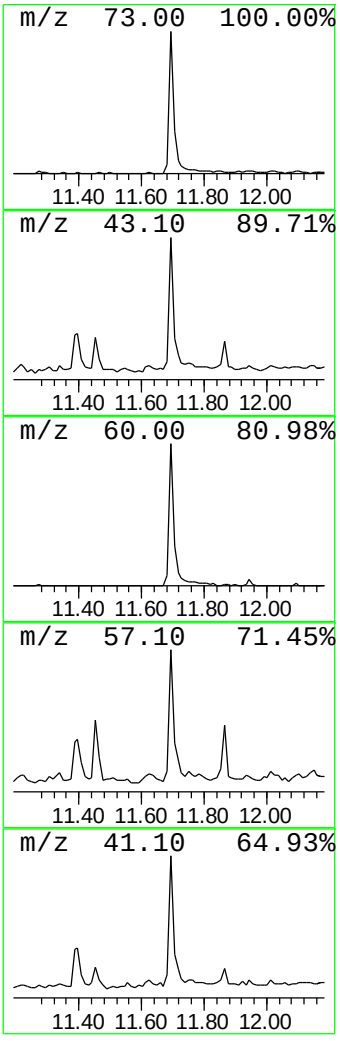
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	7.27 ng	427567	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	27





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Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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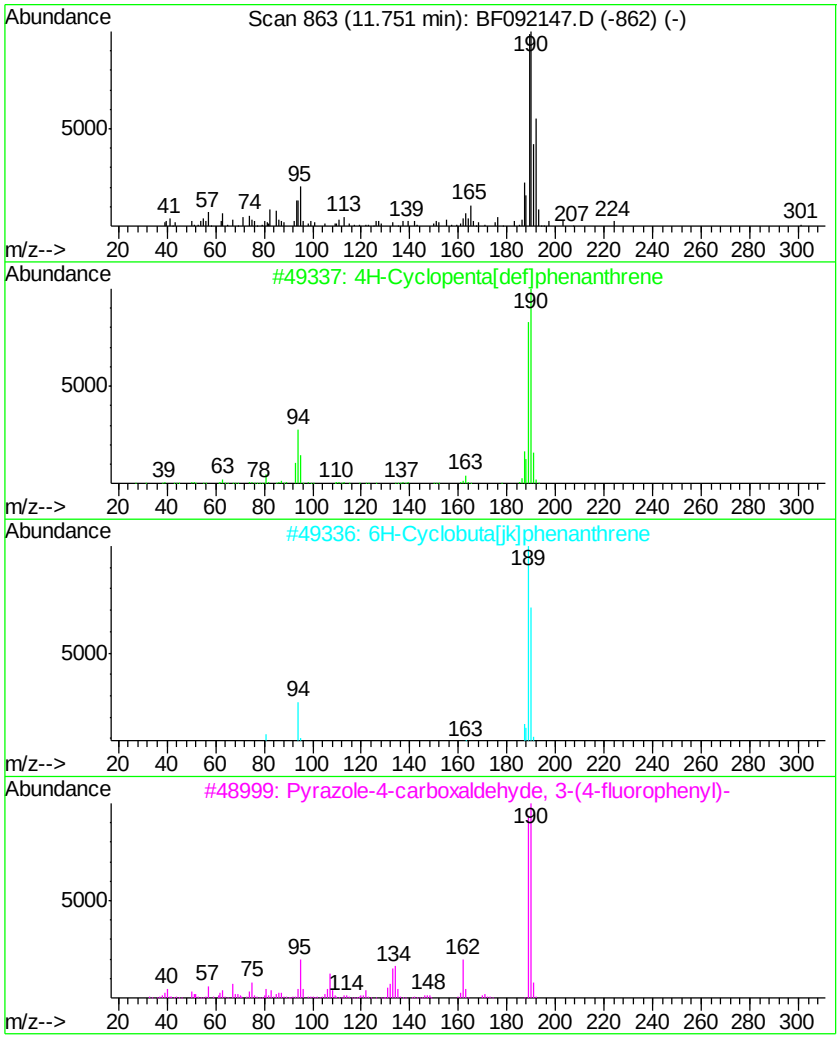
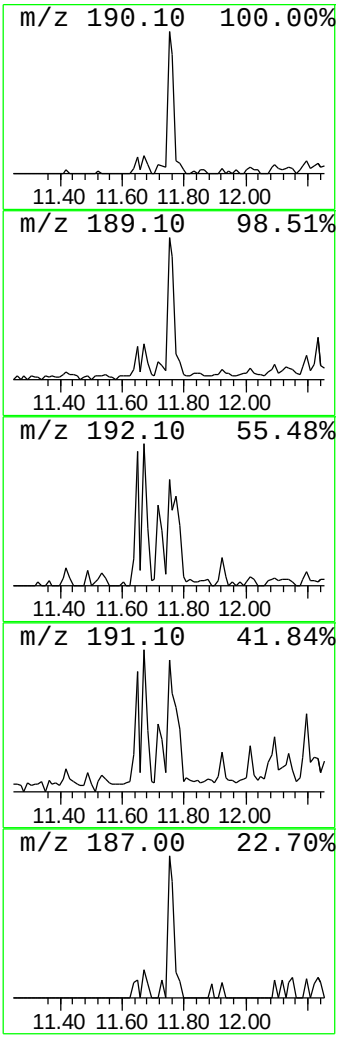
Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.78 ng	163602	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
4	3-(Trifluoromethoxy)benzaldehyde	190	C8H5F3O2	052771-21-8	43
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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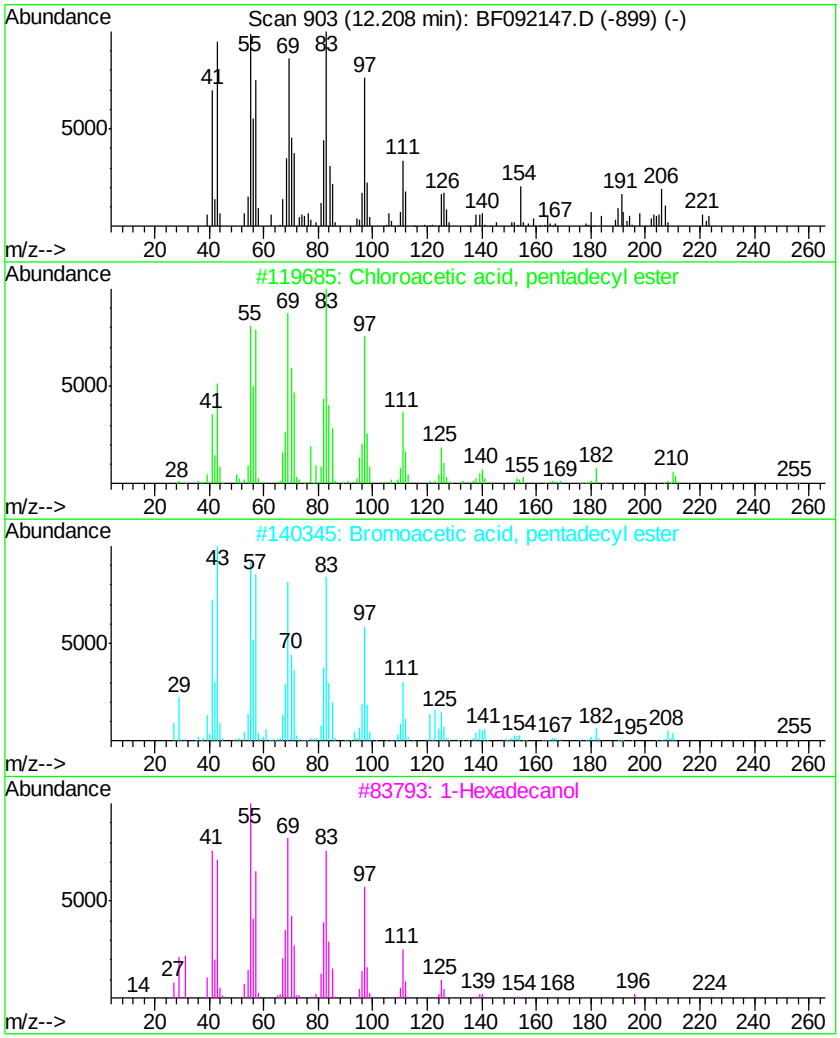
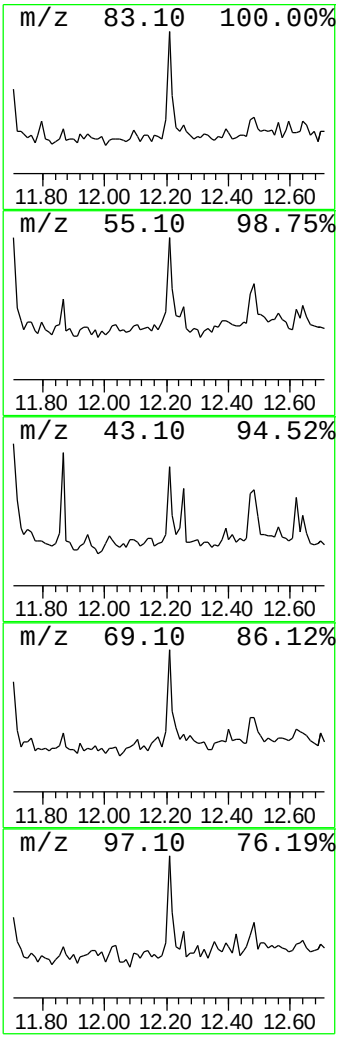
Peak Number 8 Chloroacetic acid, pentadec... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.21	2.66 ng	156407	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	93
2	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	93
3	1-Hexadecanol	242	C16H34O	036653-82-4	90
4	1-Heptadecanol	256	C17H36O	001454-85-9	90
5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87





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Data File : BF092147.D
Acq On : 9 Jan 2017 19:42
Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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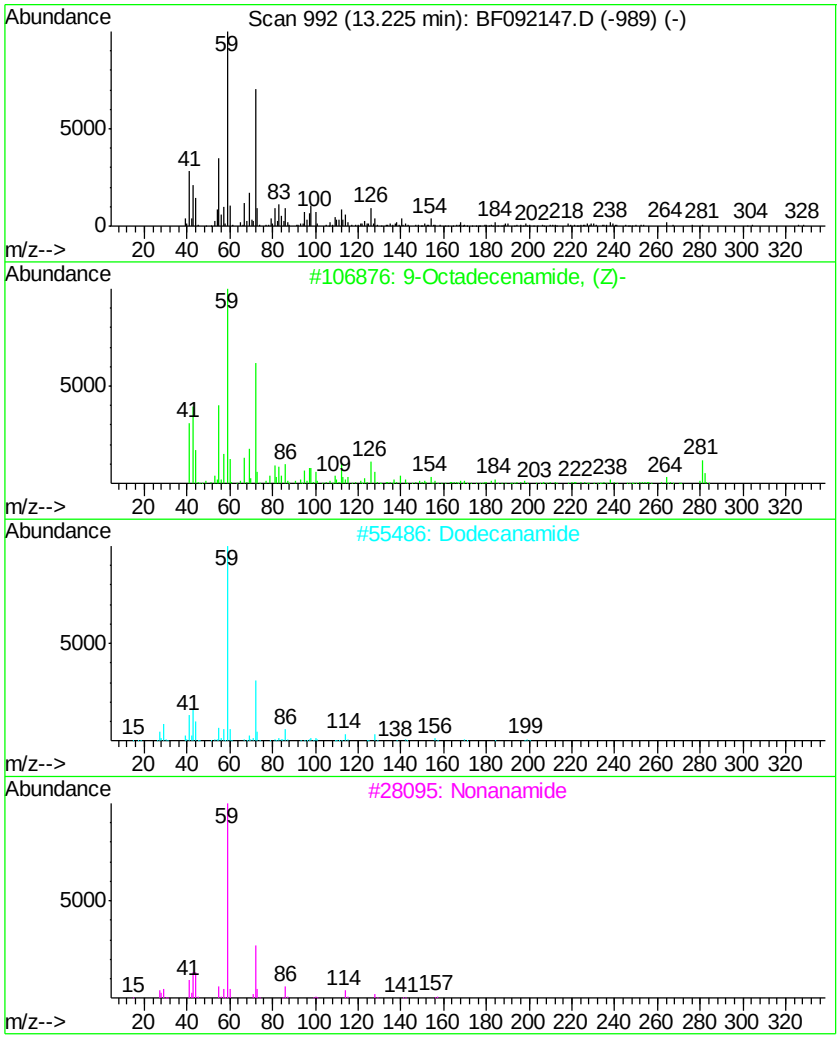
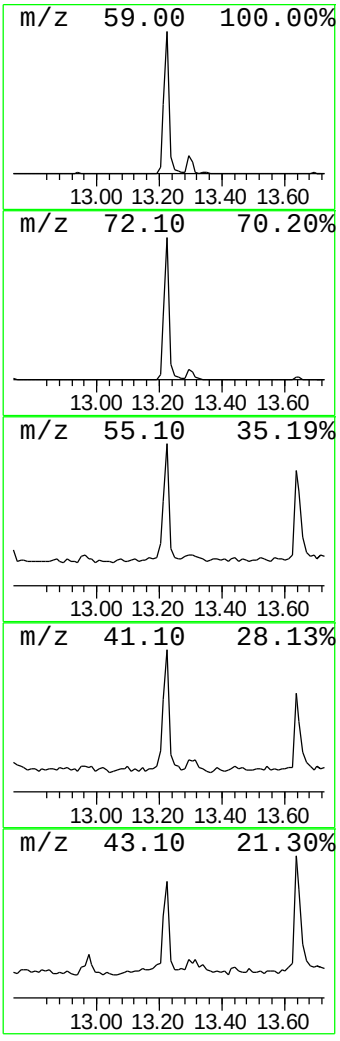
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	5.26 ng	340600	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Dodecanamide	199	C12H25NO	001120-16-7	64
3	Nonanamide	157	C9H19NO	001120-07-6	59
4	Octanamide	143	C8H17NO	000629-01-6	59
5	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	53





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Data File : BF092147.D
Acq On : 9 Jan 2017 19:42
Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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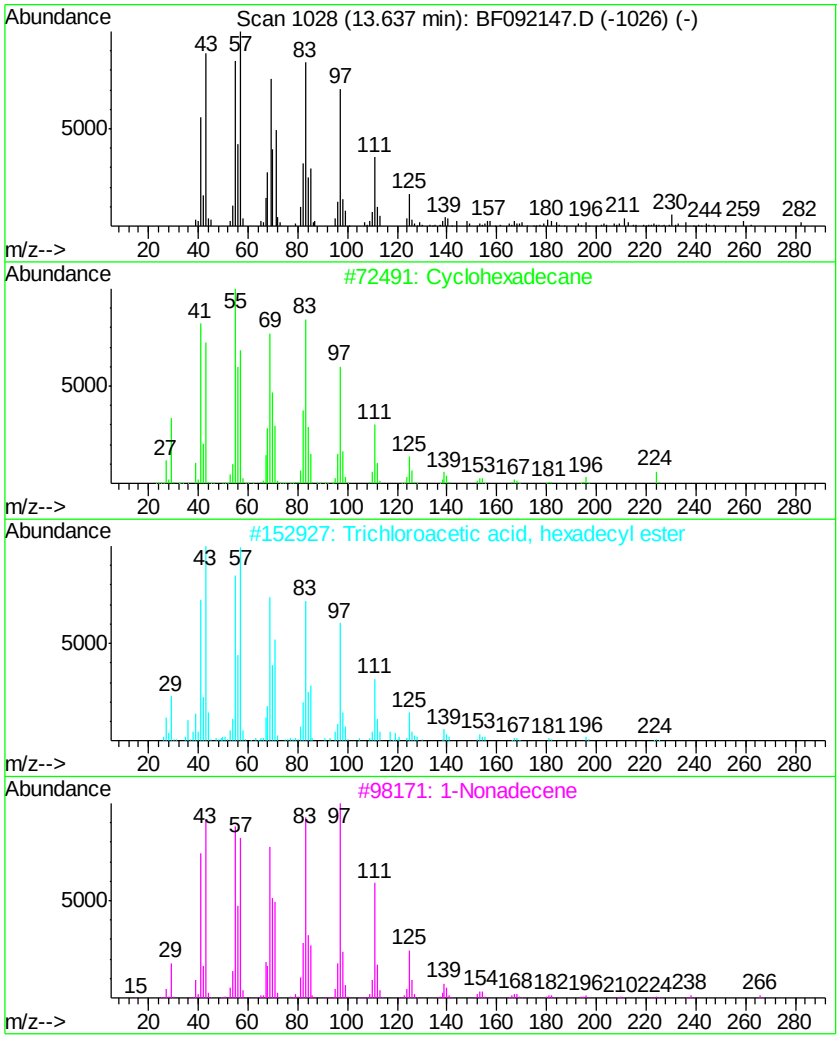
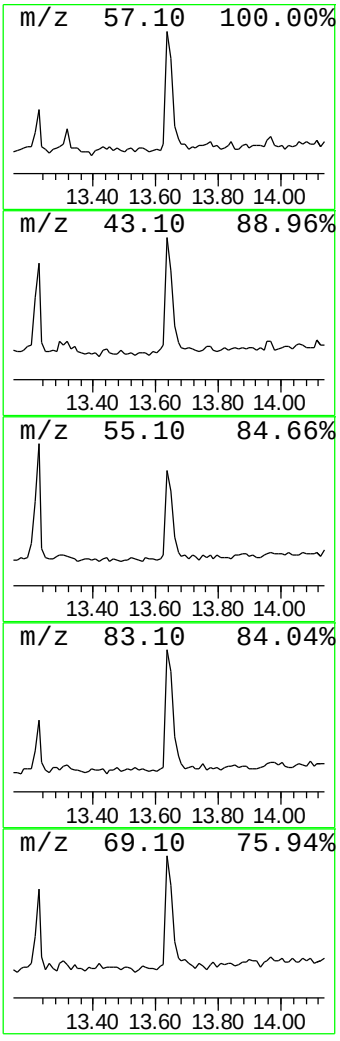
Peak Number 11 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	3.88 ng	251698	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	96
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





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Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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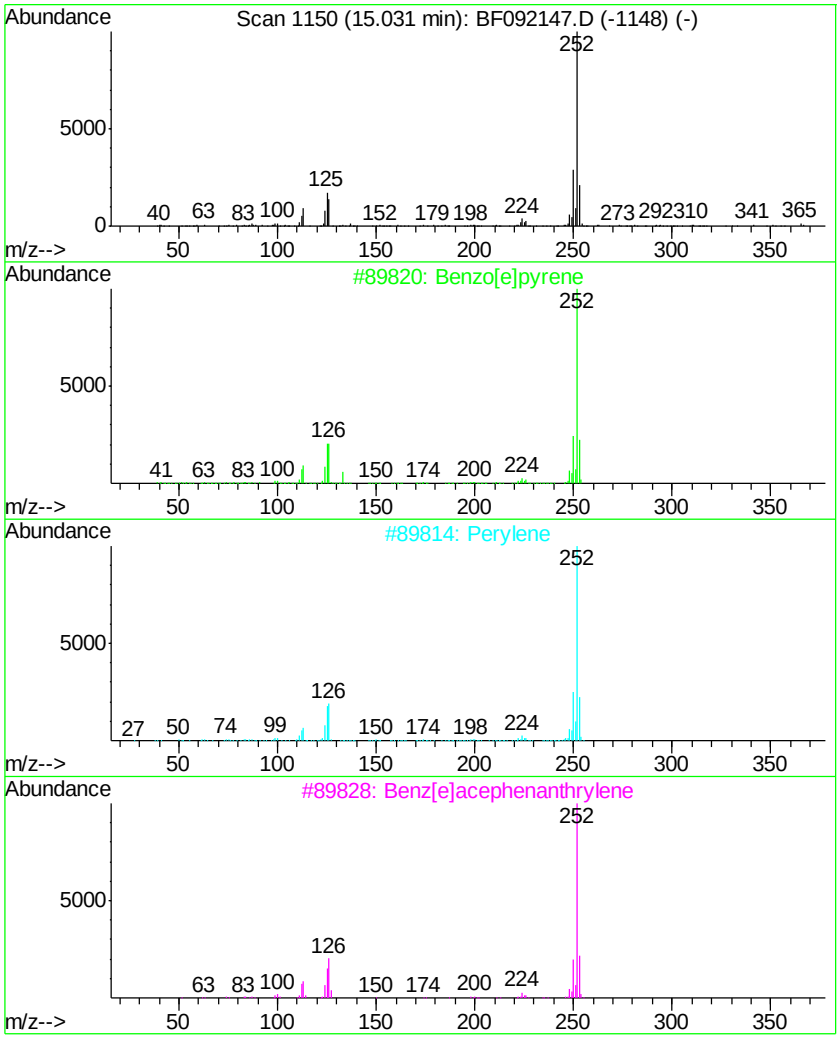
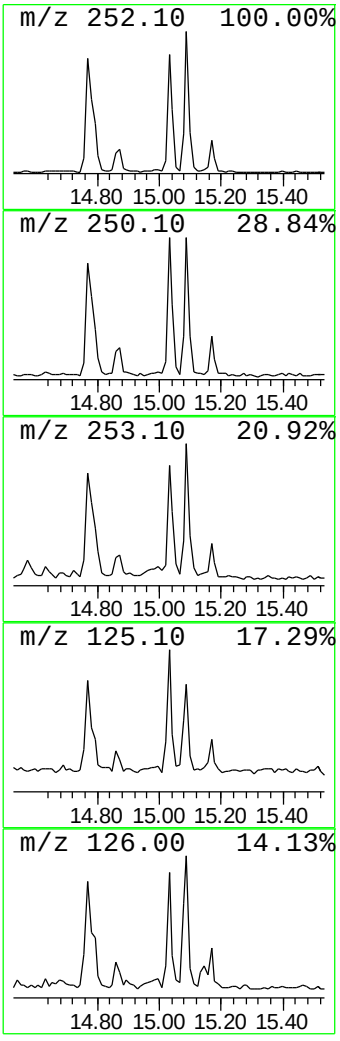
Peak Number 12 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	3.80 ng	173351	Perylene-d12	15.15

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	99
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4	Benzo[a]pyrene	252	C20H12	000050-32-8	95
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092147.D
Acq On : 9 Jan 2017 19:42
Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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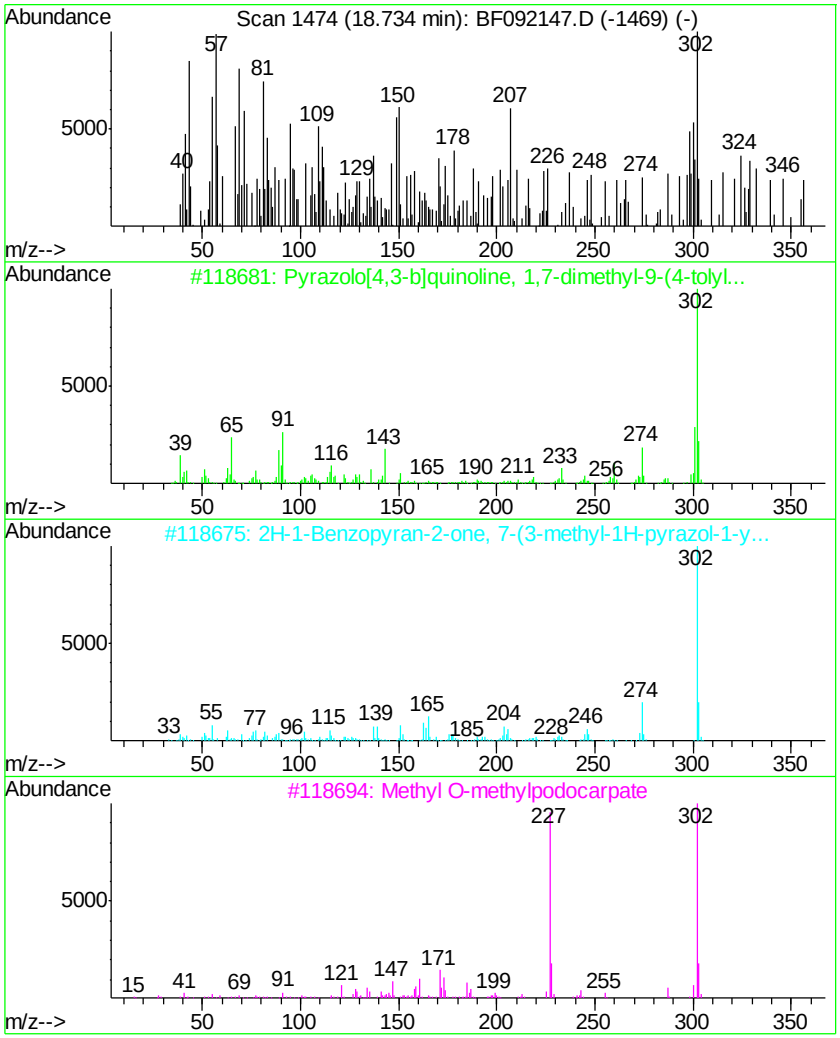
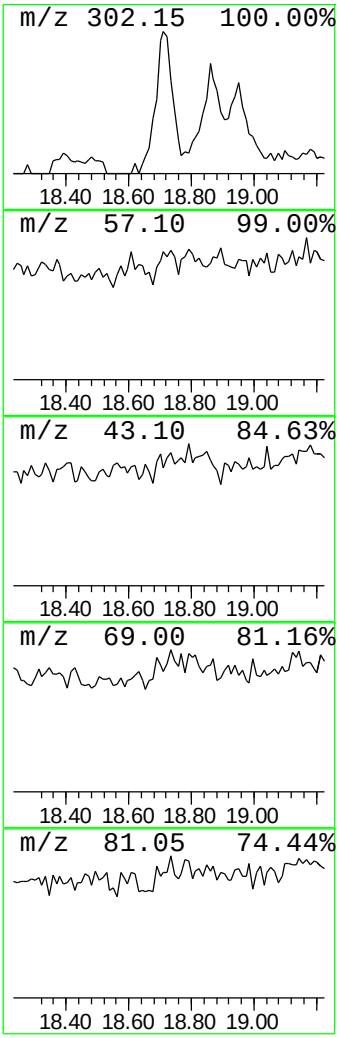
Peak Number 13 unknown18.73 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.73	3.93 ng	178976	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazolo[4,3-b]quinoline, 1,7-di...	302	C19H18N4	1000263-77-1	25
2	2H-1-Benzopyran-2-one, 7-(3-meth...	302	C19H14N2O2	006025-18-9	25
3	Methyl O-methylpodocarpate	302	C19H26O3	001231-74-9	25
4	5H-Indano[1,2-c]pyridazin-5-one,...	302	C18H10N2O3	329720-51-6	25
5	6,7-Dihydro-3,3-dimethyl-6-(3,4-...	302	C16H14O6	1000242-76-7	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092147.D
Acq On : 9 Jan 2017 19:42
Operator : UM/SJ
Sample : I1064-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP4-COMP12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.77	49.0	ng	2427910	1	6.63	990641	20.0
unknown6.40	6.40	95.6	ng	4733050	1	6.63	990641	20.0
Benzenesulfonamid...	10.57	5.0	ng	293371	4	11.14	1176960	20.0
1-Pentadecene	11.40	3.2	ng	186618	4	11.14	1176960	20.0
n-Hexadecanoic acid	11.69	7.3	ng	427567	4	11.14	1176960	20.0
4H-Cyclopenta[def...	11.75	2.8	ng	163602	4	11.14	1176960	20.0
Chloroacetic acid...	12.21	2.7	ng	156407	4	11.14	1176960	20.0
9-Octadecenamide,...	13.23	5.3	ng	340600	5	13.77	1295830	20.0
Cyclohexadecane	13.64	3.9	ng	251698	5	13.77	1295830	20.0
Benzo[e]pyrene	15.03	3.8	ng	173351	6	15.15	911450	20.0
unknown18.73	18.73	3.9	ng	178976	6	15.15	911450	20.0