LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088628.D
Acq On : 2 Jul 2016 20:33
Operator : UM/SJ
Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

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-BF063016.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	1.861	19	24	33	rVB	53054	86817	2.97%	0.329%
2	2.993	122	123	129	rBV2	31934	74073	2.54%	0.281%
3	4.284	233	236	239	rBB	40386	51254	1.75%	0.194%
4	4.959	292	295	304	rBB	165109	238963	8.18%	0.906%
5	5.393	330	333	335	rBV	2154925	2741084	93.82%	10.396%
6	6.433	421	424	426	rBV	2399680	2921527	100.00%	11.080%
7	6.559	432	435	438	rBV	2553869	2455922	84.06%	9.314%
8	6.787	453	455	457	rBV	543183	666300	22.81%	2.527%
9	6.947	467	469	472	rVB	2054938	1918709	65.67%	7.277%
10	7.359	502	505	507	rBV	1884191	1827783	62.56%	6.932%
11	7.450	511	513	516	rBV	26721	38727	1.33%	0.147%
12	8.079	566	568	570	rBV	1100457	918109	31.43%	3.482%
13	9.153	660	662	665	rBV	2355480	2556725	87.51%	9.697%
14	9.553	695	697	699	rBV	600460	565770	19.37%	2.146%
15	9.828	719	721	723	rBV	1013836	873207	29.89%	3.312%
16	10.273	759	760	762	rVB	52792	36775	1.26%	0.139%
17	10.616	787	790	792	rBV	1403334	1441461	49.34%	5.467%
18	10.742	800	801	805	rVB	56417	61035	2.09%	0.231%
19	11.188	839	840	846	rVB	101702	125934	4.31%	0.478%
20	11.302	848	850	854	rVB2	656730	903367	30.92%	3.426%
21	11.382	854	857	858	rBV3	67766	83040	2.84%	0.315%
22	11.531	869	870	875	rVB3	24423	44476	1.52%	0.169%
23	11.622	875	878	885	rVB	63017	113831	3.90%	0.432%
24	11.805	893	894	895	rBV	40588	30706	1.05%	0.116%
25	11.839	895	897	899	rVV2	64960	77863	2.67%	0.295%
26	11.873	899	900	902	rVB2	40552	45716	1.56%	0.173%
27	11.919	902	904	908	rVB2	53996	83941	2.87%	0.318%
28	12.102	918	920	924	rVB3	26082	41334	1.41%	0.157%
29	12.514	954	956	958	rBV	354052	306898	10.50%	1.164%
30	12.742	973	976	977	rBV	235752	312532	10.70%	1.185%
31	12.788	977	980	983	rVB4	13671	36126	1.24%	0.137%
32	12.891	987	989	991	rVV	1931265	1703420	58.31%	6.460%
33	12.959	991	995	999	rVB2	22262	34235	1.17%	0.130%
34	13.062	1001	1004	1006	rVB	31939	61881	2.12%	0.235%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.131	1006	1010	1012	rBV	32893	52901	1.81%	0.201%
36	13.165	1012	1013	1017	rVV2	34181	47583	1.63%	0.180%
37	13.474	1035	1040	1043	rBV6	15942	45281	1.55%	0.172%
38	13.565	1046	1048	1051	rVB	29890	43089	1.47%	0.163%
39	13.679	1056	1058	1060	rBV	34448	64116	2.19%	0.243%
40	13.794	1065	1068	1072	rVV3	127286	175996	6.02%	0.667%
41	13.931	1077	1080	1086	rVB2	773819	993888	34.02%	3.769%
42	14.319	1109	1114	1115	rBV	42477	87154	2.98%	0.331%
43	14.434	1120	1124	1129	rVV6	21878	99635	3.41%	0.378%
44	14.788	1154	1155	1158	rVB	43774	38700	1.32%	0.147%
45	14.937	1165	1168	1173	rBV	132534	273277	9.35%	1.036%
46	15.211	1190	1192	1195	rVB	74903	94187	3.22%	0.357%
47	15.268	1195	1197	1200	rBV	103171	122833	4.20%	0.466%
48	15.325	1200	1202	1205	rBV	375285	582977	19.95%	2.211%
49	16.663	1316	1319	1325	rBV2	39874	82516	2.82%	0.313%
50	17.063	1351	1354	1363	rVB	33110	83179	2.85%	0.315%

Sum of corrected areas: 26366853

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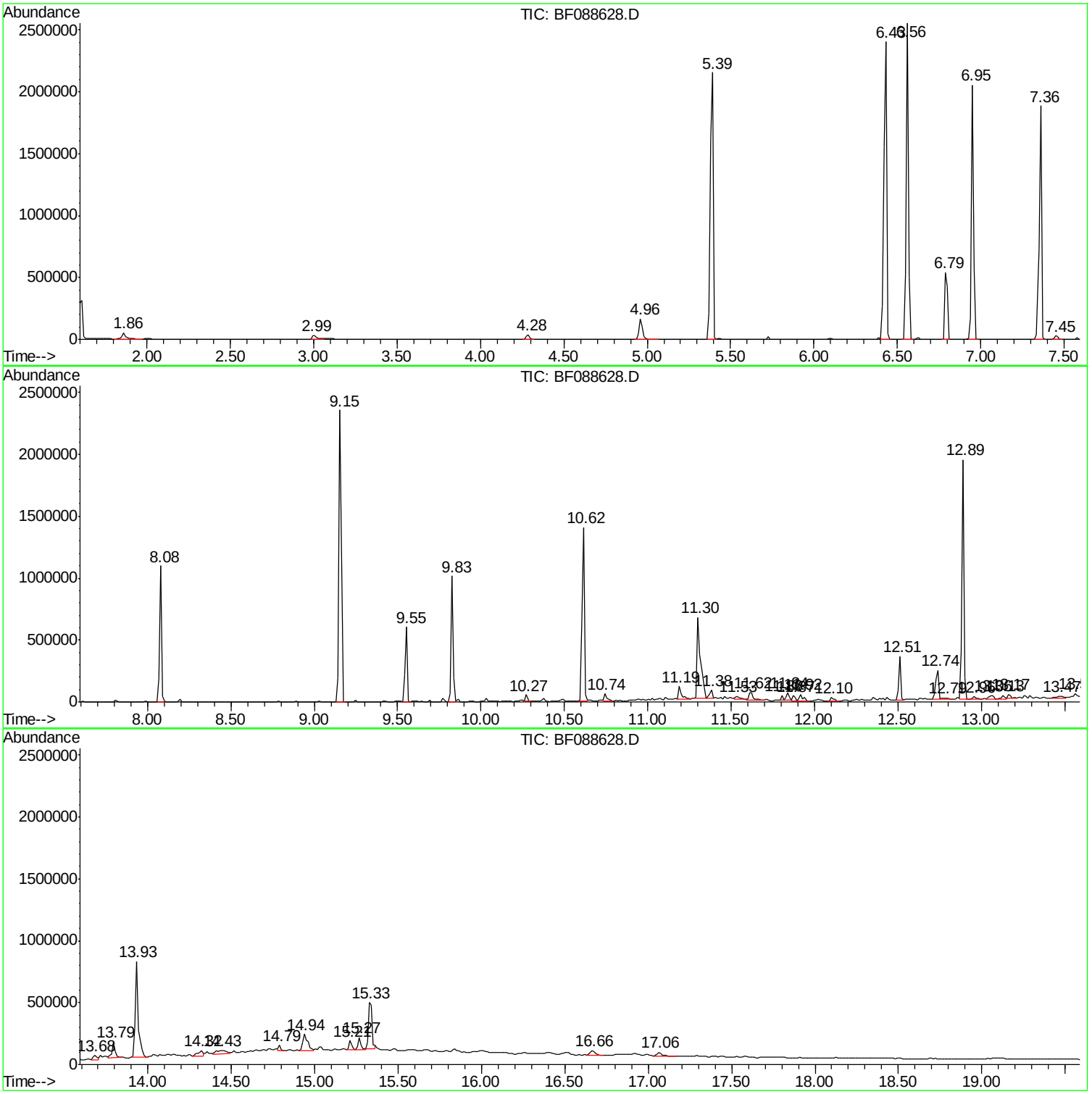
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF088628.D
Acq On : 2 Jul 2016 20:33
Operator : UM/SJ
Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

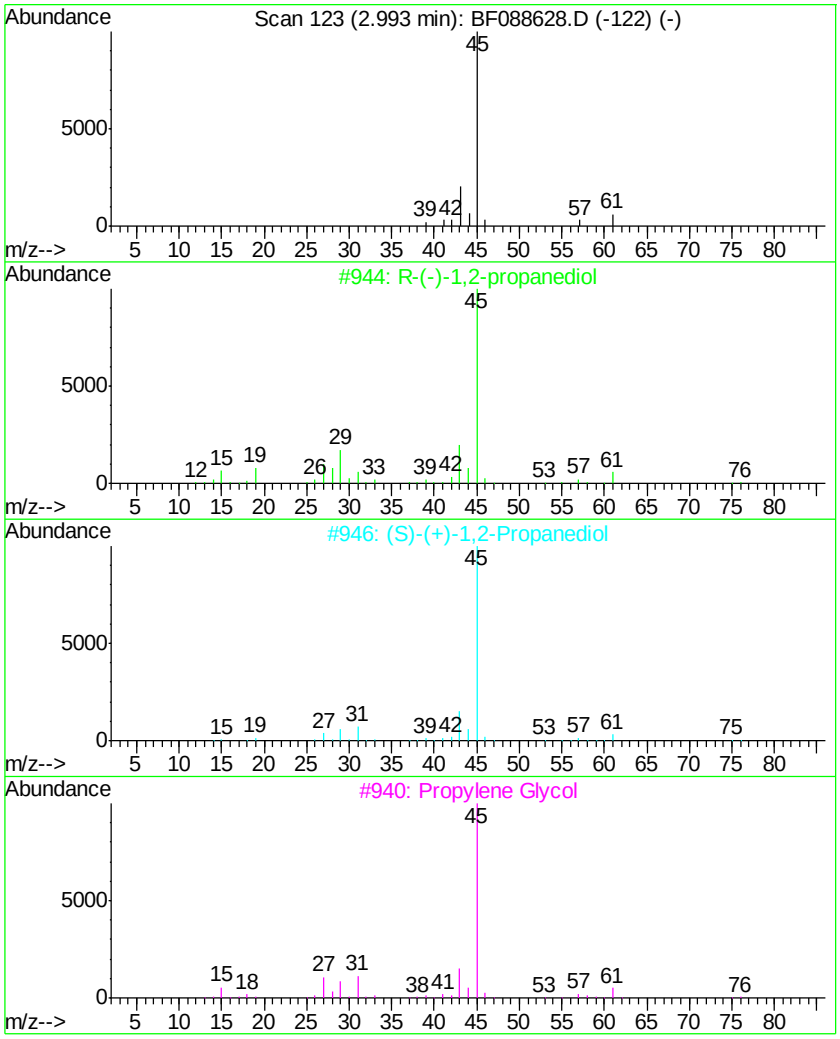
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

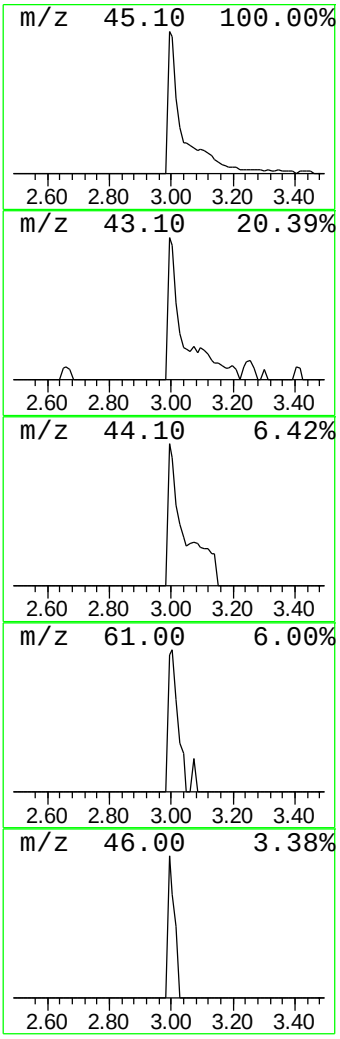
****

Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	2.22 ng	74073	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Formamide	45	CH3NO	000075-12-7	5
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	4





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Operator : UM/SJ
Sample : H3847-11
Misc :
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Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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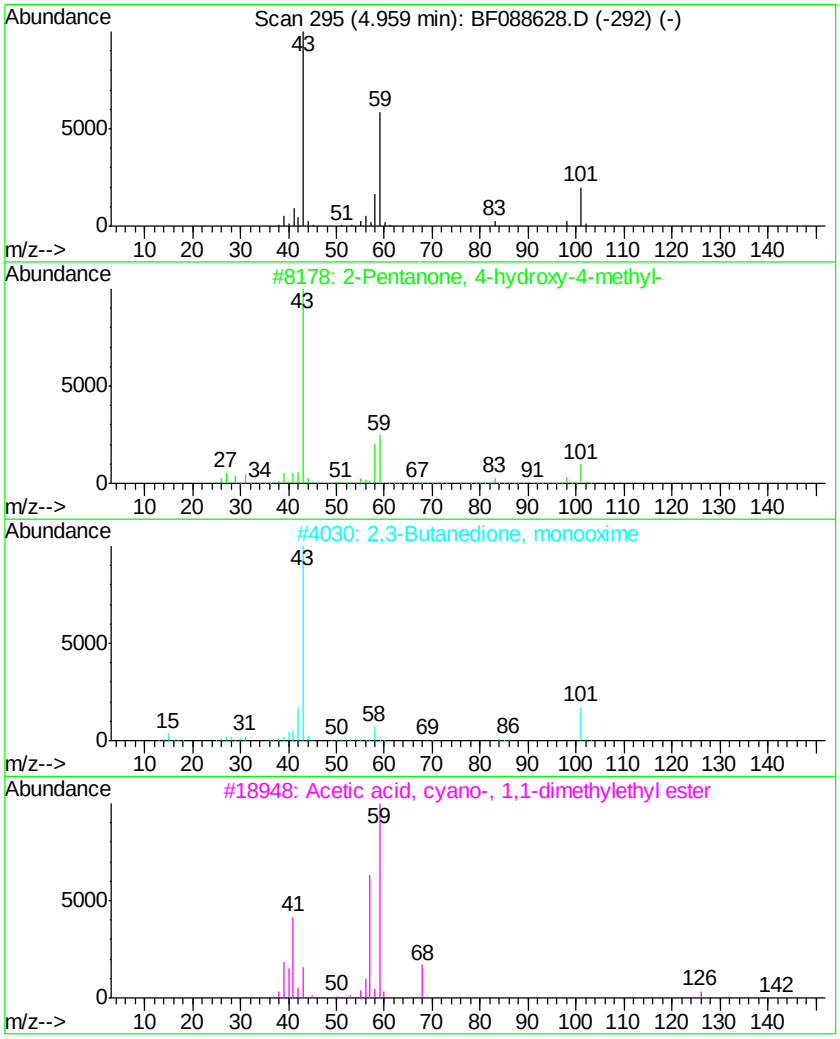
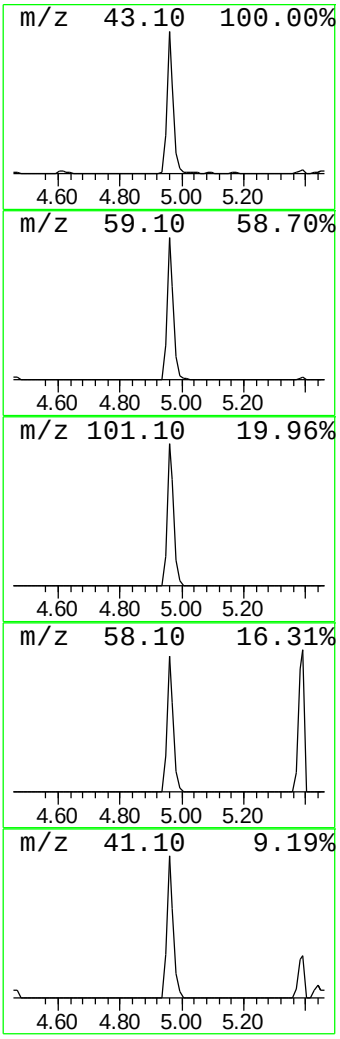
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	7.17 ng	238963	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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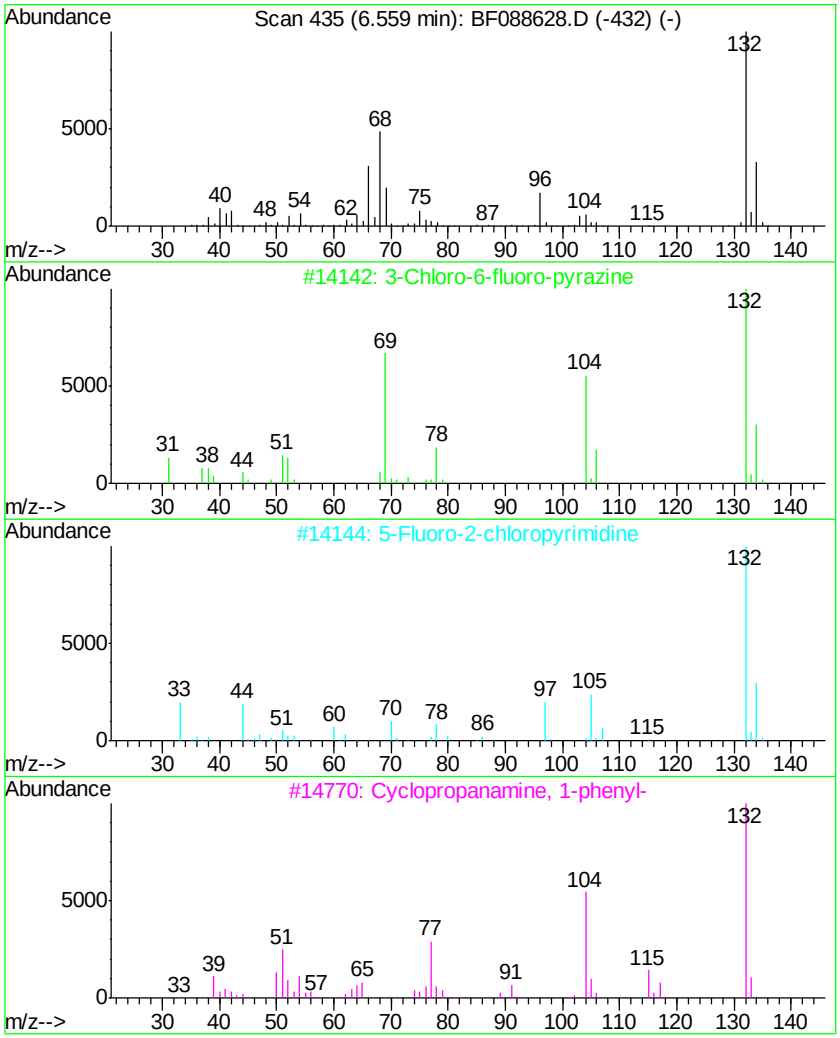
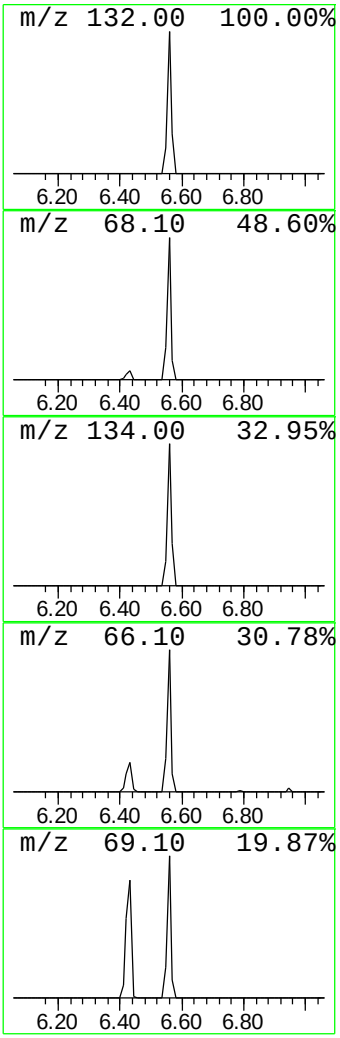
Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	73.72 ng	2455920	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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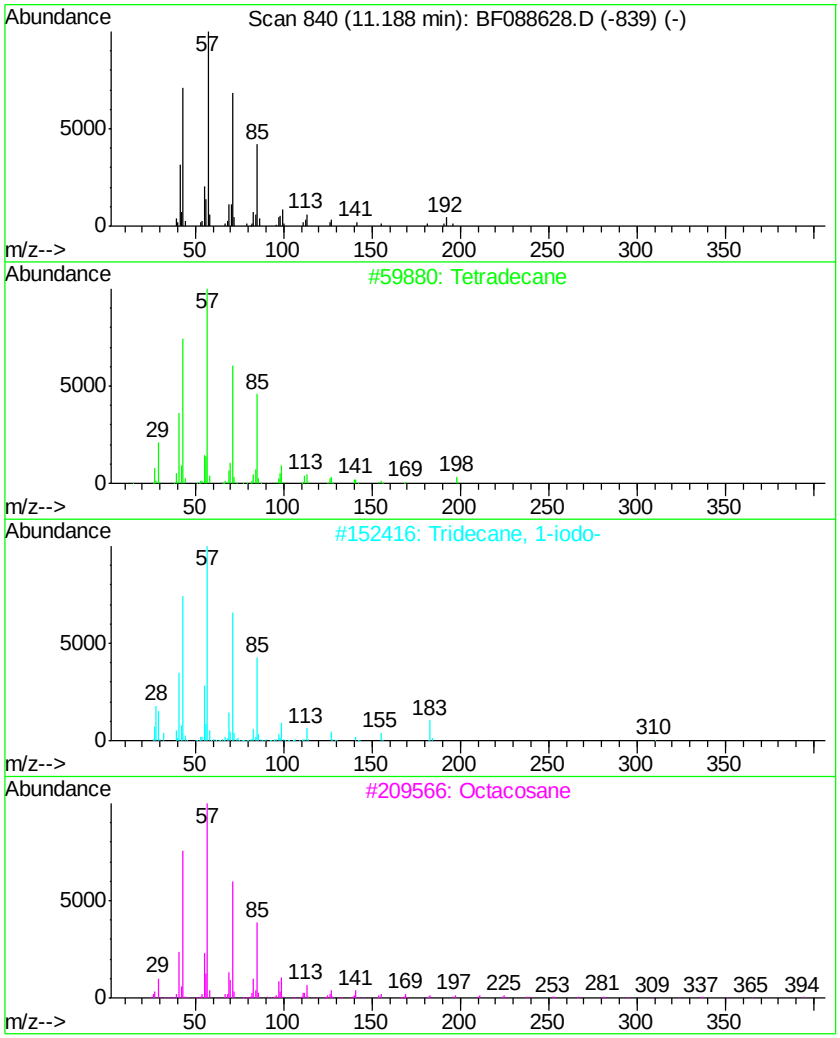
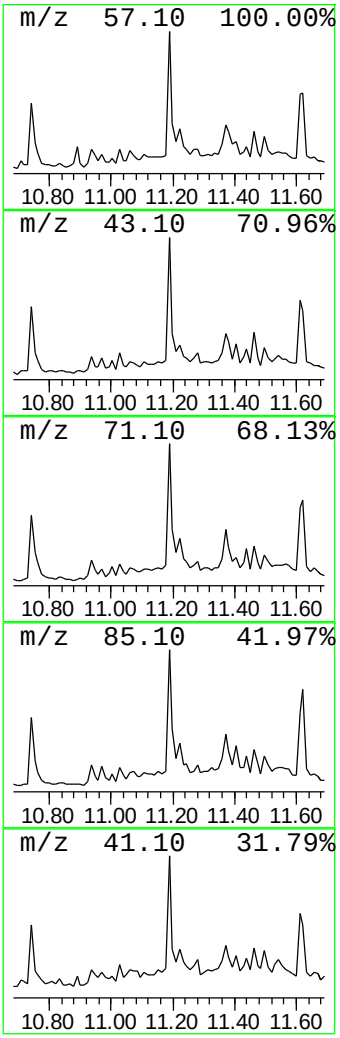
Peak Number 6 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.79 ng	125934	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	87
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3	Octacosane	394	C28H58	000630-02-4	86
4	Hexadecane	226	C16H34	000544-76-3	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





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Operator : UM/SJ
Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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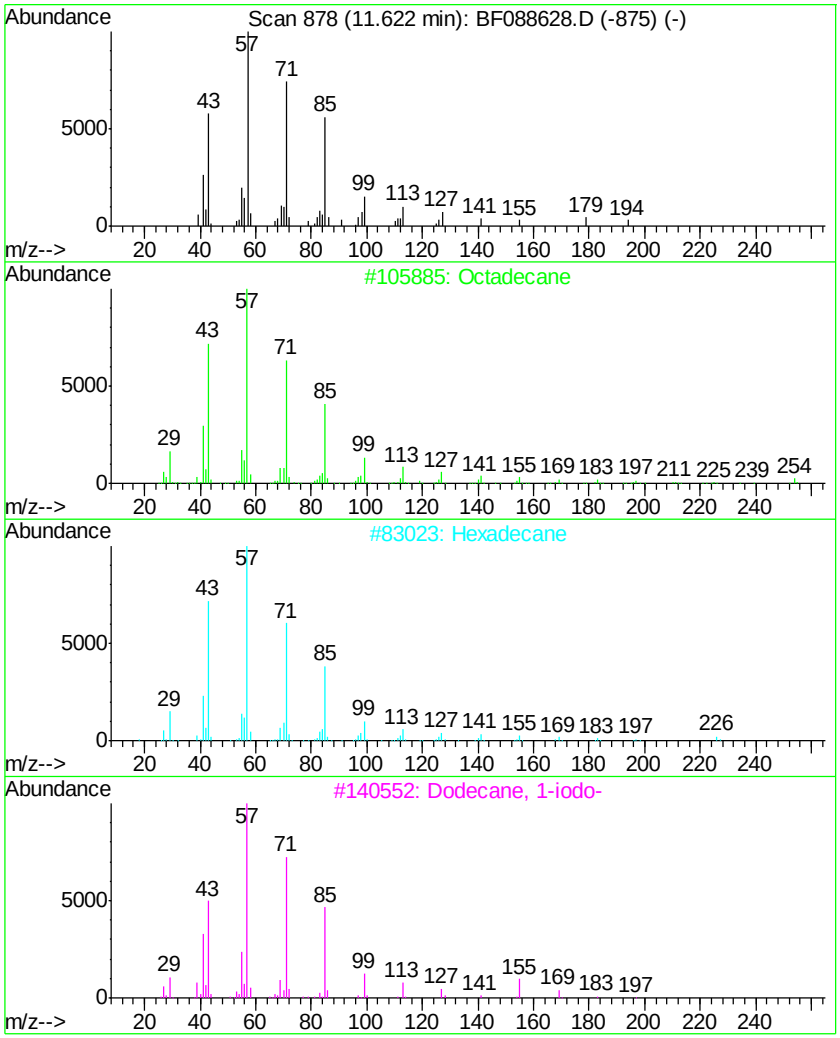
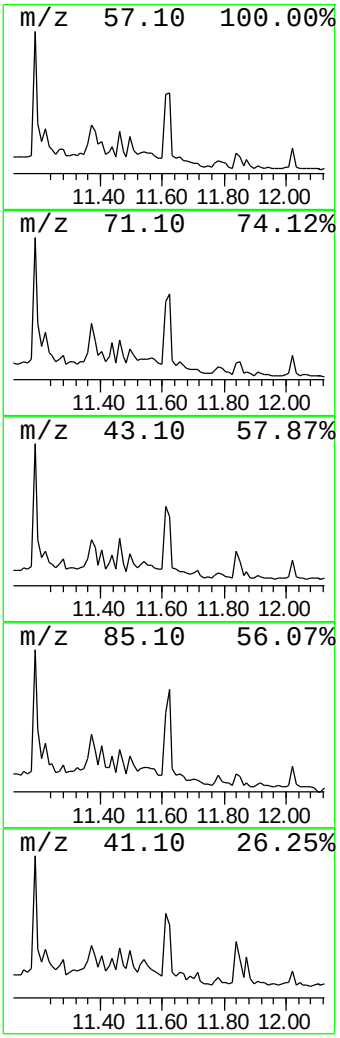
Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.62	2.52 ng	113831	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Heptadecane	240	C17H36	000629-78-7	80
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72





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Data File : BF088628.D
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Operator : UM/SJ
Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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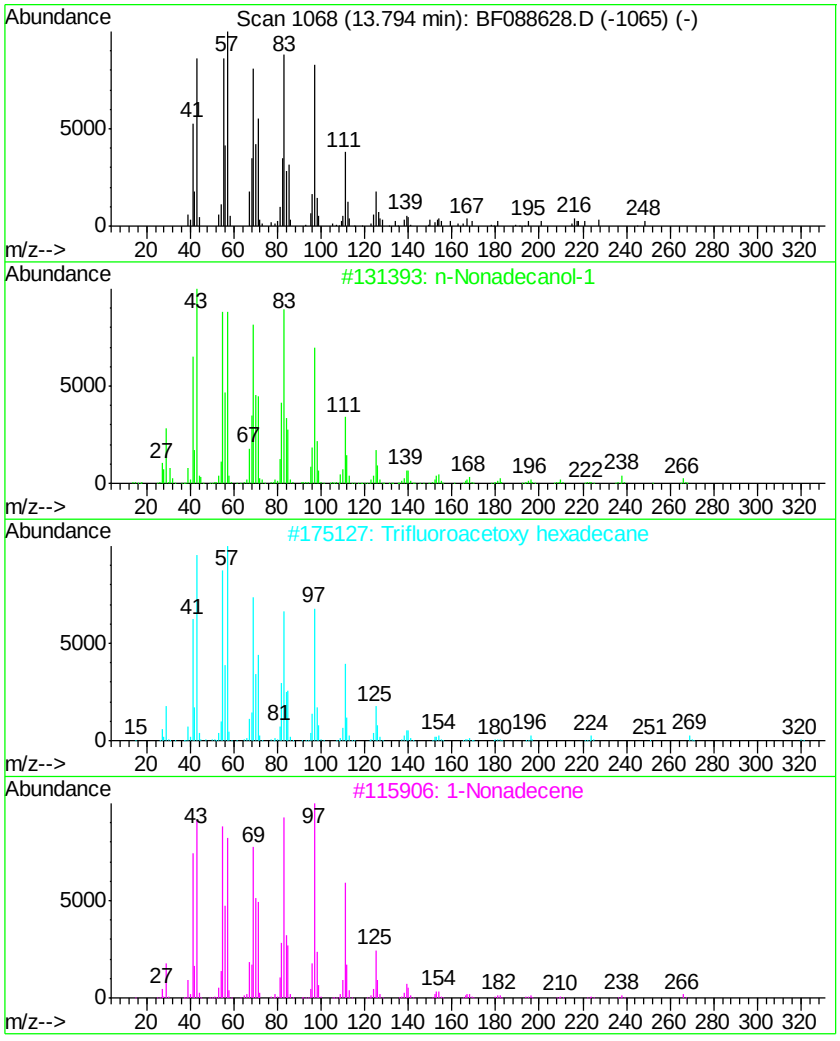
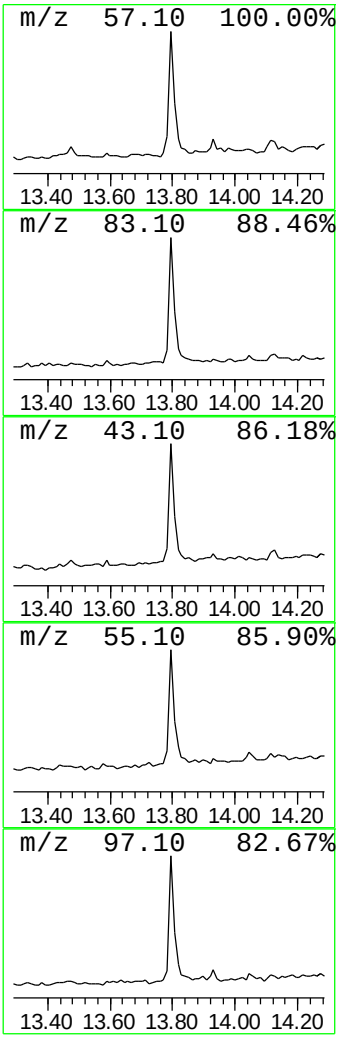
Peak Number 8 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.54 ng	175996	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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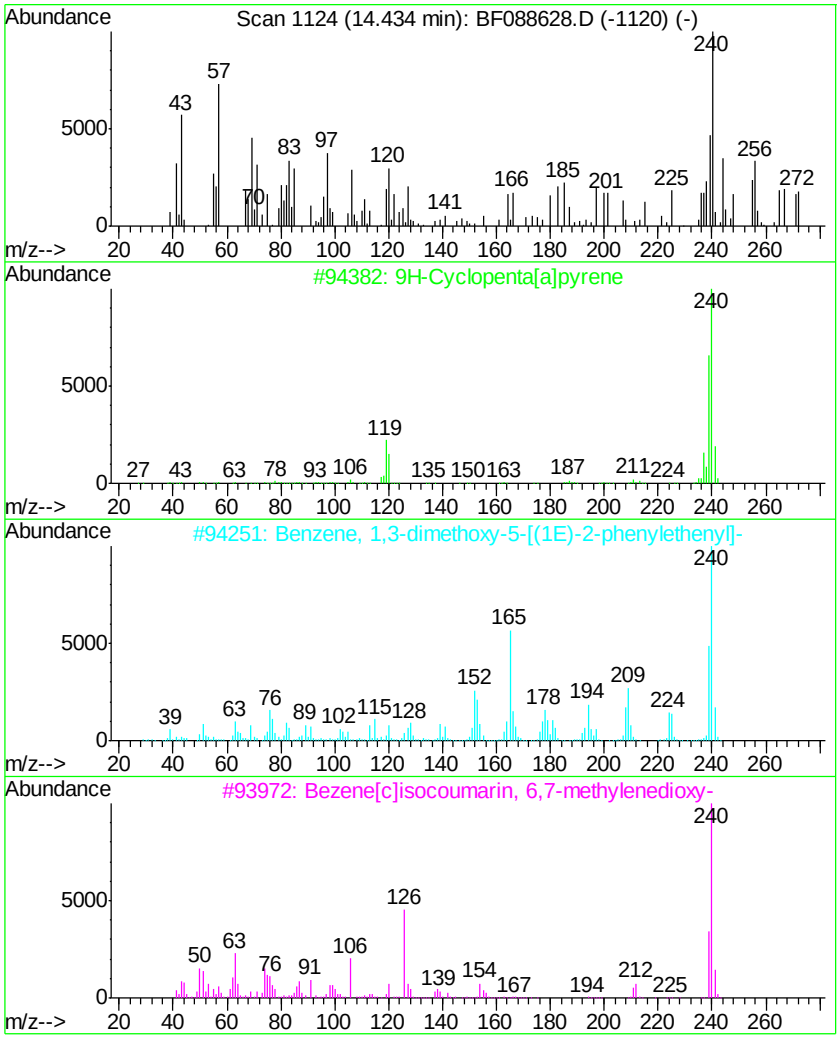
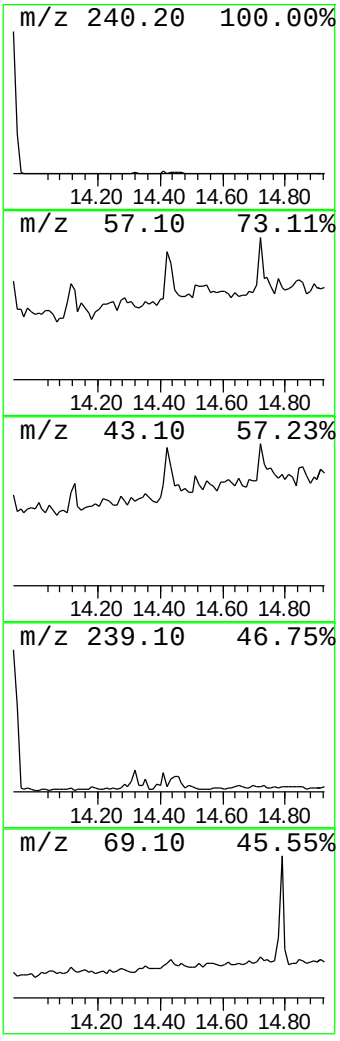
Peak Number 9 unknown14.43 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	2.00 ng	99635	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Cyclopenta[a]pyrene	240	C19H12	050861-05-7	32
2	Benzene, 1,3-dimethoxy-5-[(1E)-2...	240	C16H16O2	021956-56-9	25
3	Bezene[c]isocoumarin, 6,7-methyl...	240	C14H8O4	004445-35-6	25
4	3,4,5-Trimethoxy-2-methylbenzoic...	240	C12H16O5	247180-24-1	18
5	[1,1'-Biphenyl]-4,4'-diamine, 3,...	240	C16H20N2	054827-17-7	18





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Operator : UM/SJ
Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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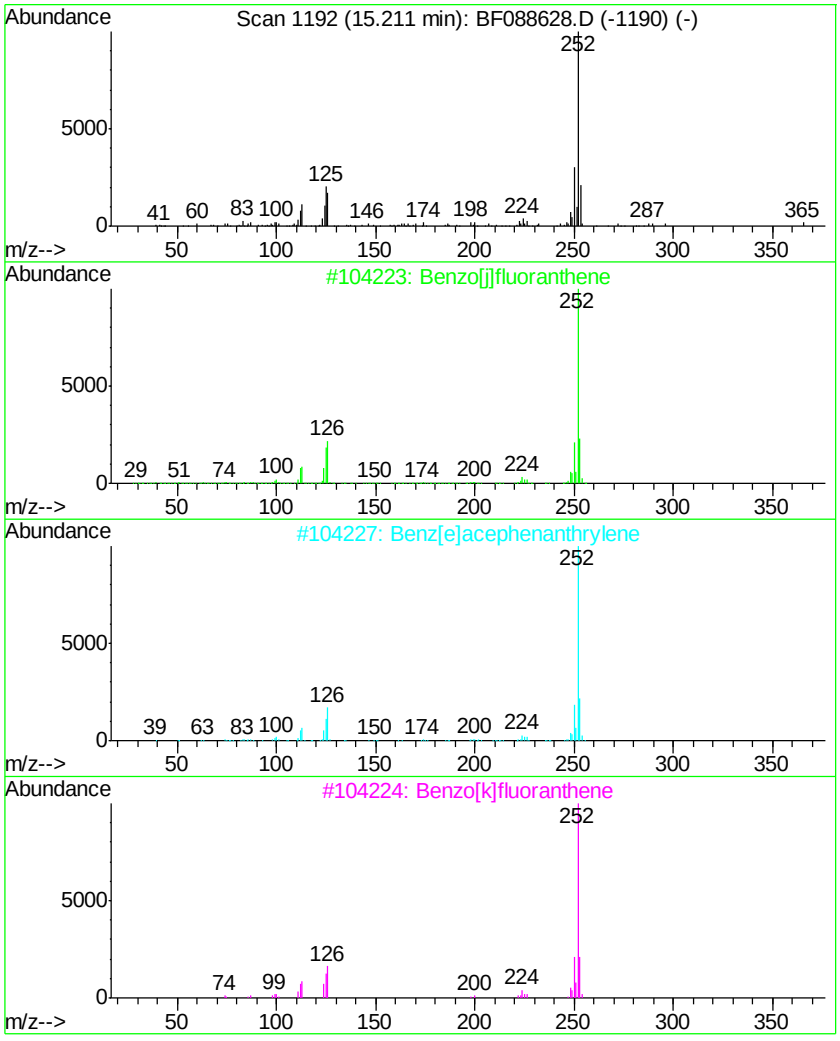
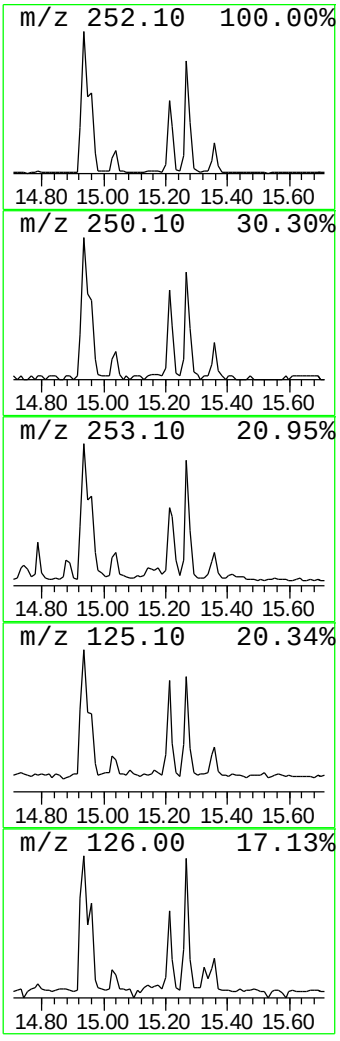
Peak Number 10 Benzo[j]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	3.23 ng	94187	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[e]pyrene	252	C20H12	000192-97-2	93
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088628.D
Acq On : 2 Jul 2016 20:33
Operator : UM/SJ
Sample : H3847-11
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B1(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
R-(-)-1,2-propane...	2.99	2.2	ng	74073	1	6.80	666300	20.0
2-Pentanone, 4-hy...	4.96	7.2	ng	238963	1	6.80	666300	20.0
unknown6.56	6.56	73.7	ng	2455920	1	6.80	666300	20.0
Tetradecane	11.19	2.8	ng	125934	4	11.30	903367	20.0
Octadecane	11.62	2.5	ng	113831	4	11.30	903367	20.0
n-Nonadecanol-1	13.79	3.5	ng	175996	5	13.93	993888	20.0
unknown14.43	14.43	2.0	ng	99635	5	13.93	993888	20.0
Benzo[j]fluoranthene	15.21	3.2	ng	94187	6	15.34	582977	20.0