LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088626.D
Acq On : 2 Jul 2016 19:35
Operator : UM/SJ
Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(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	1.724	10	12	22	rVB	74295	155827	6.30%	0.580%
2	1.861	22	24	52	rVB	640786	1355711	54.80%	5.045%
3	3.004	120	124	133	rBV	93227	214803	8.68%	0.799%
4	4.273	233	235	238	rVB	35673	52303	2.11%	0.195%
5	4.958	292	295	299	rBV	160005	206545	8.35%	0.769%
6	5.381	329	332	335	rBV	1962826	2202973	89.05%	8.198%
7	6.067	389	392	393	rBV	58700	54959	2.22%	0.205%
8	6.421	421	423	426	rVB	1705804	2473875	100.00%	9.206%
9	6.490	428	429	432	rVB	52880	49477	2.00%	0.184%
10	6.559	432	435	437	rBV	2517091	2346945	94.87%	8.734%
11	6.787	453	455	457	rVB	593821	691912	27.97%	2.575%
12	6.947	467	469	471	rVB	1989450	1813777	73.32%	6.750%
13	7.359	502	505	507	rVB	1735112	1711599	69.19%	6.370%
14	7.450	510	513	516	rBV	35135	42756	1.73%	0.159%
15	7.987	555	560	562	rBV3	27749	43069	1.74%	0.160%
16	8.079	565	568	570	rBV	1197787	1011839	40.90%	3.766%
17	8.433	595	599	601	rBV4	17415	50737	2.05%	0.189%
18	8.525	604	607	611	rVV4	24436	48777	1.97%	0.182%
19	8.627	614	616	618	rBV	28121	30579	1.24%	0.114%
20	8.867	635	637	640	rVB3	19280	30328	1.23%	0.113%
21	9.153	660	662	665	rBV	2339321	2366539	95.66%	8.807%
22	9.245	667	670	672	rBV	31527	35585	1.44%	0.132%
23	9.553	695	697	699	rVB	742106	691642	27.96%	2.574%
24	9.690	707	709	712	rBV	29872	42075	1.70%	0.157%
25	9.770	715	716	719	rBV	30970	37811	1.53%	0.141%
26	9.828	719	721	723	rVB	1099178	931595	37.66%	3.467%
27	10.273	759	760	762	rVB	50527	35012	1.42%	0.130%
28	10.616	787	790	792	rBV	1111315	1284253	51.91%	4.779%
29	10.742	800	801	805	rVB	56651	63013	2.55%	0.235%
30	11.188	839	840	842	rBV	105944	103399	4.18%	0.385%
31	11.302	848	850	854	rVB	766474	830075	33.55%	3.089%
32	11.382	854	857	858	rBV3	53306	77894	3.15%	0.290%
33	11.542	869	871	875	rVB3	26525	56417	2.28%	0.210%
34	11.611	875	877	881	rVB	66842	97009	3.92%	0.361%

LSC Area Percent Report

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Acq On : 2 Jul 2016 19:35
Operator : UM/SJ
Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(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	11.839	895	897	899	rBV2	69073	88935	3.59%	0.331%
36	11.919	902	904	908	rVB	34607	51298	2.07%	0.191%
37	12.102	919	920	924	rVB3	16261	30468	1.23%	0.113%
38	12.411	944	947	948	rBV2	22714	26283	1.06%	0.098%
39	12.514	954	956	958	rBV	271342	250755	10.14%	0.933%
40	12.559	958	960	963	rBV4	11358	24931	1.01%	0.093%
41	12.628	965	966	968	rBV2	18588	25005	1.01%	0.093%
42	12.742	973	976	978	rVV	161699	262282	10.60%	0.976%
43	12.788	978	980	985	rVB4	15810	25427	1.03%	0.095%
44	12.891	987	989	991	rVV	1799667	1593612	64.42%	5.931%
45	12.959	991	995	999	rVB3	25760	45456	1.84%	0.169%
46	13.062	1001	1004	1008	rBV2	33479	86141	3.48%	0.321%
47	13.131	1008	1010	1012	rVB	30891	30393	1.23%	0.113%
48	13.165	1012	1013	1015	rBV	37679	48333	1.95%	0.180%
49	13.256	1019	1021	1023	rBV2	21017	29052	1.17%	0.108%
50	13.394	1031	1033	1036	rVB	25559	35749	1.45%	0.133%
51	13.474	1036	1040	1042	rBV5	22903	60785	2.46%	0.226%
52	13.565	1046	1048	1053	rVB	28819	48668	1.97%	0.181%
53	13.679	1056	1058	1060	rBV	32684	59905	2.42%	0.223%
54	13.794	1067	1068	1072	rVB3	114394	143837	5.81%	0.535%
55	13.931	1077	1080	1086	rVB2	785140	989349	39.99%	3.682%
56	14.034	1087	1089	1091	rBV2	34502	49067	1.98%	0.183%
57	14.319	1112	1114	1115	rVB	28673	30928	1.25%	0.115%
58	14.354	1115	1117	1119	rBV2	30253	29680	1.20%	0.110%
59	14.445	1122	1125	1128	rVB3	42814	101858	4.12%	0.379%
60	14.788	1153	1155	1157	rVB2	41716	38859	1.57%	0.145%
61	14.937	1165	1168	1173	rBV	177291	340938	13.78%	1.269%
62	15.039	1175	1177	1182	rVV2	41381	99275	4.01%	0.369%
63	15.211	1190	1192	1195	rVB	87563	121709	4.92%	0.453%
64	15.268	1195	1197	1199	rBV	112457	123927	5.01%	0.461%
65	15.337	1200	1203	1205	rBV	409438	579290	23.42%	2.156%
66	16.674	1317	1320	1323	rVB2	35200	70257	2.84%	0.261%
67	17.074	1352	1355	1359	rVB	40622	87536	3.54%	0.326%

Sum of corrected areas: 26871098

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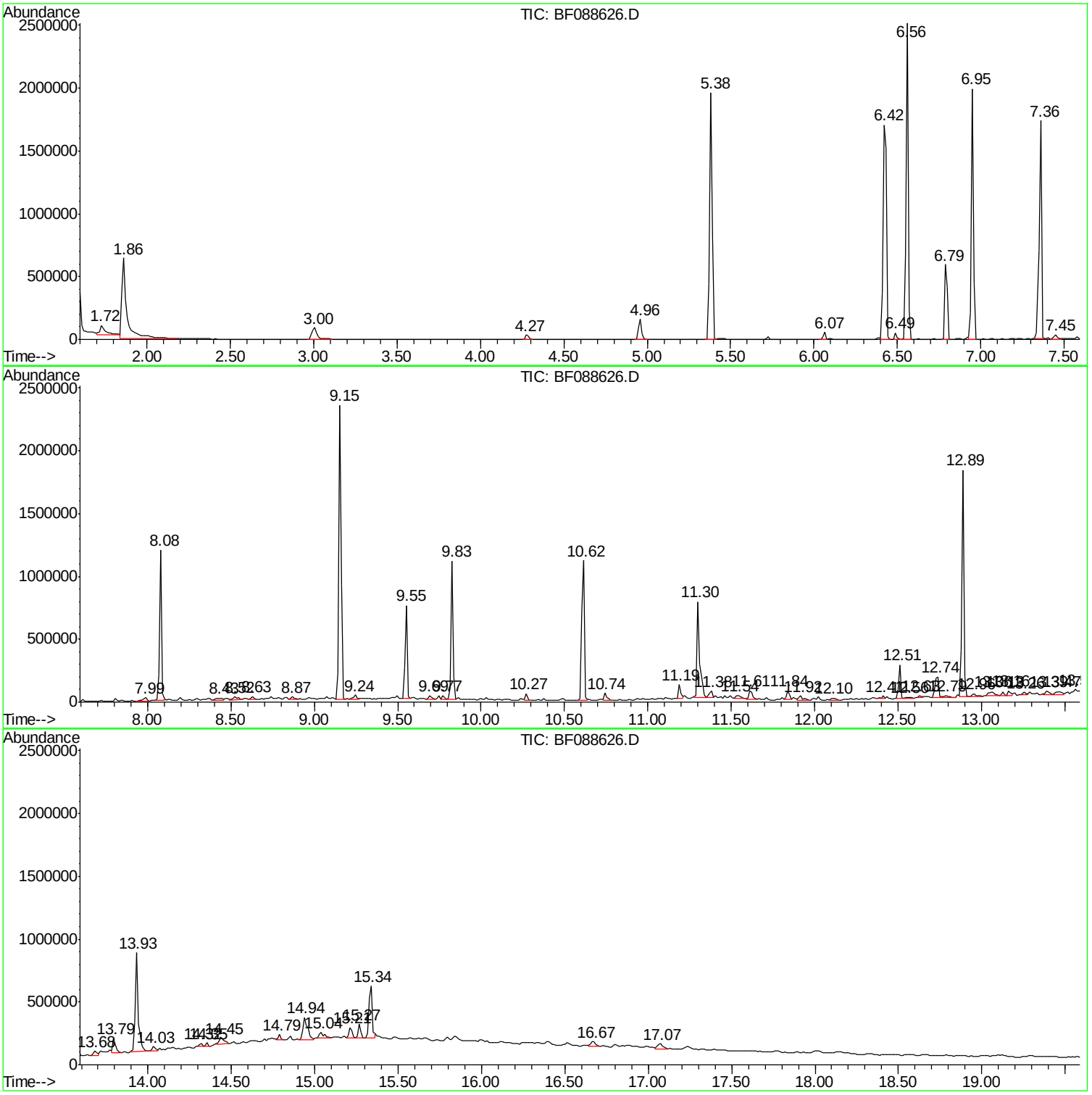
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B2(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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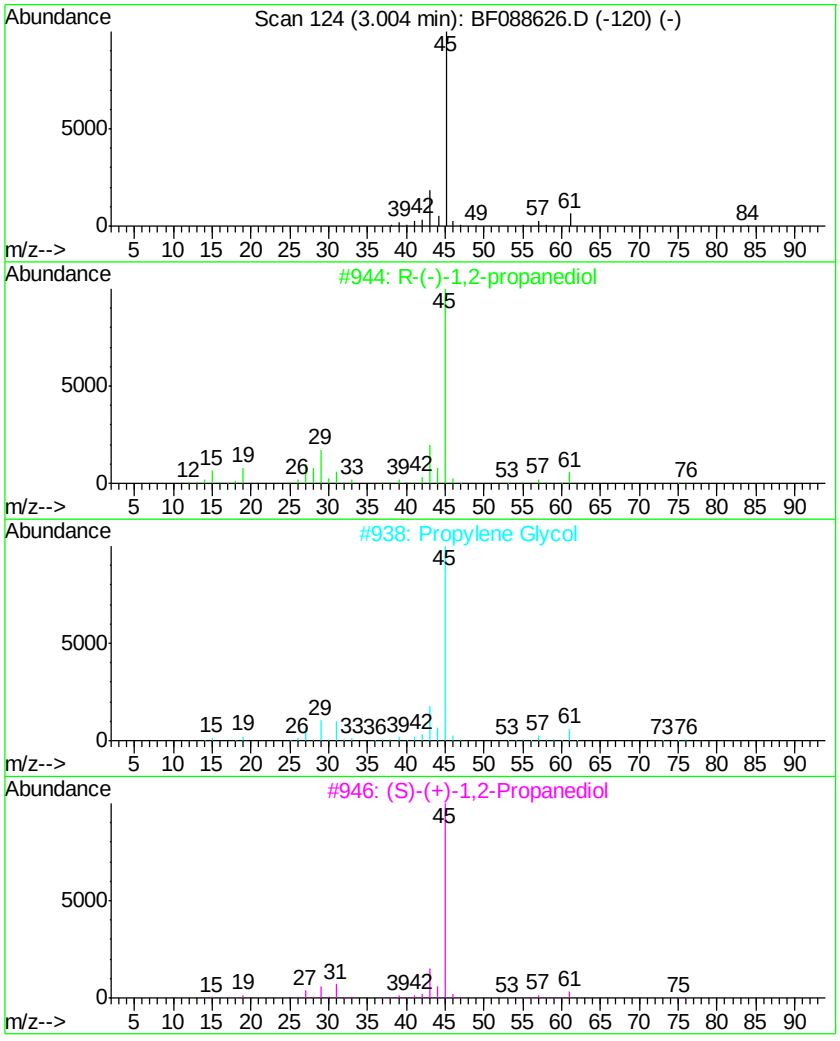
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

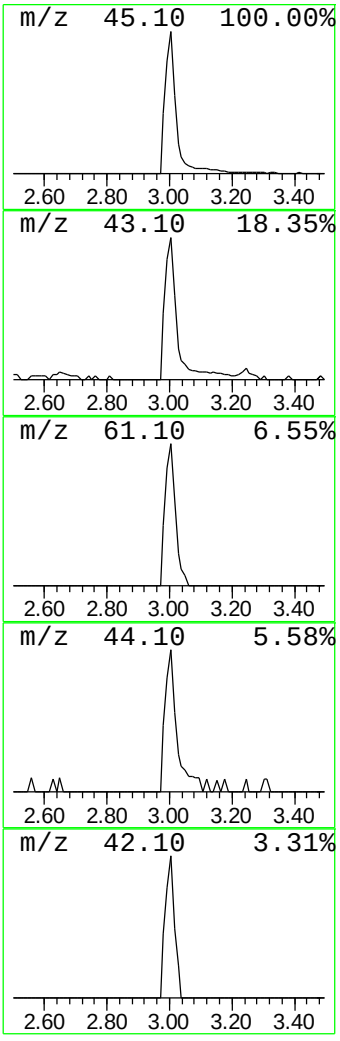
****

Peak Number 3 unknown3.00 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	6.21 ng	214803	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	43
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	2-Butanol	74	C4H10O	000078-92-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088626.D
Acq On : 2 Jul 2016 19:35
Operator : UM/SJ
Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(0-11)C

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

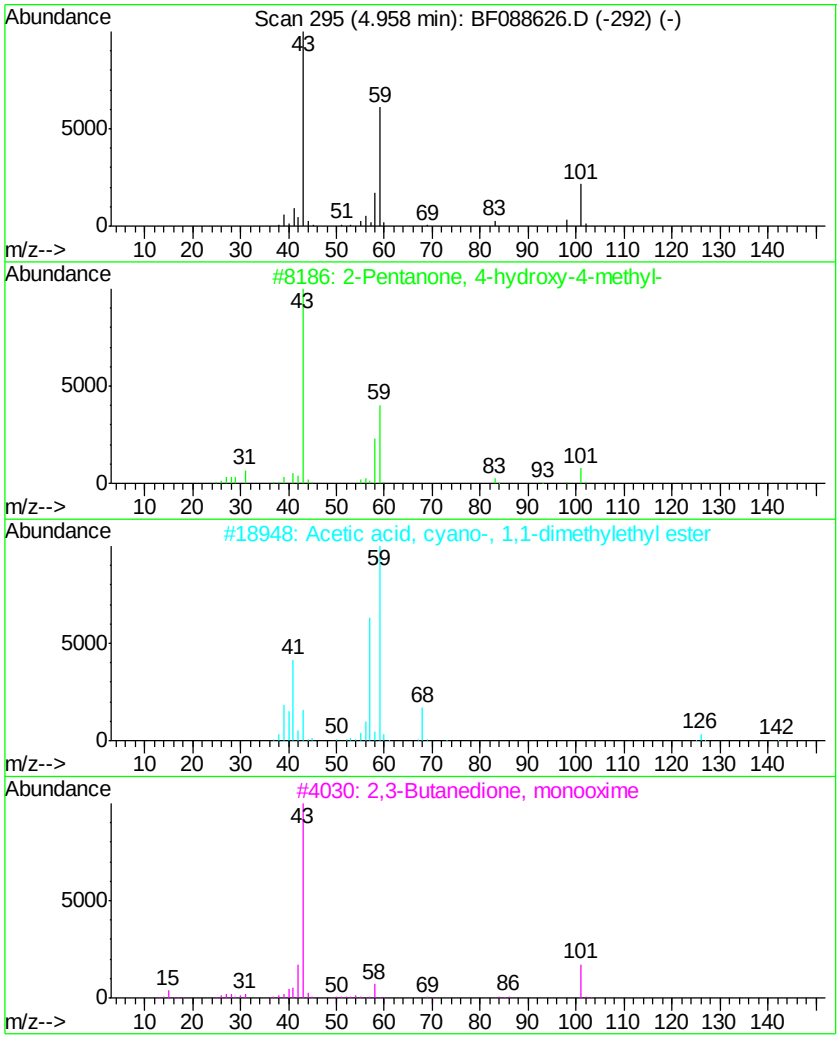
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

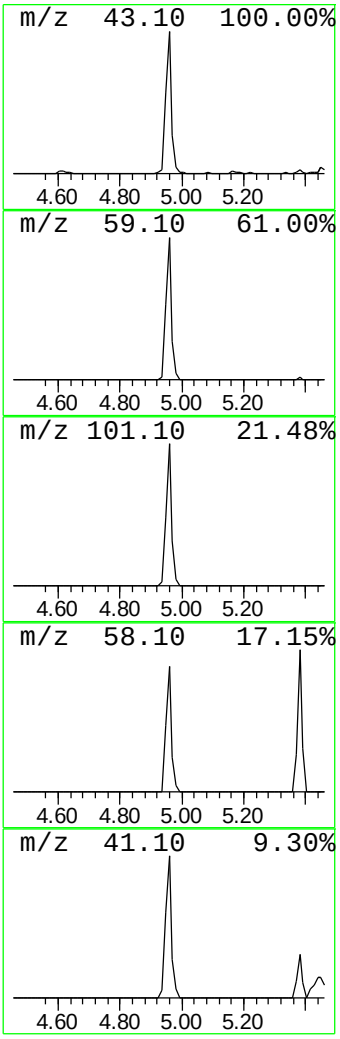
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	5.97 ng	206545	1,4-Dichlorobenzene-d4	6.79

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	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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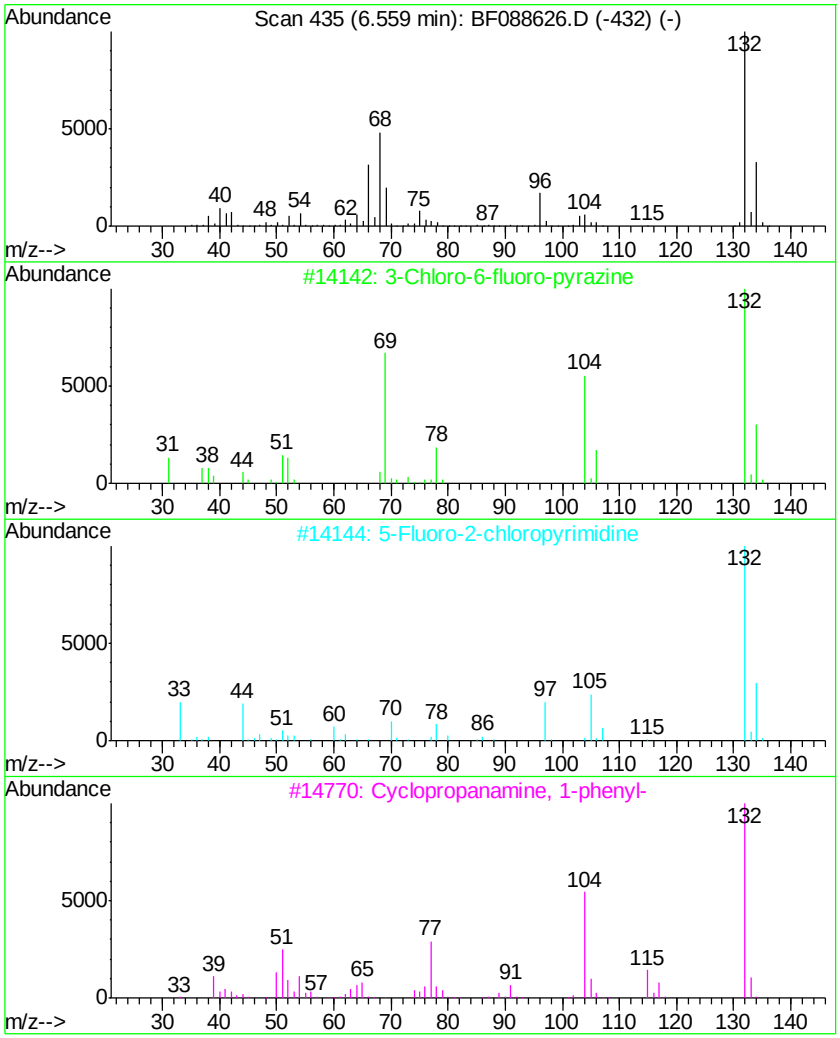
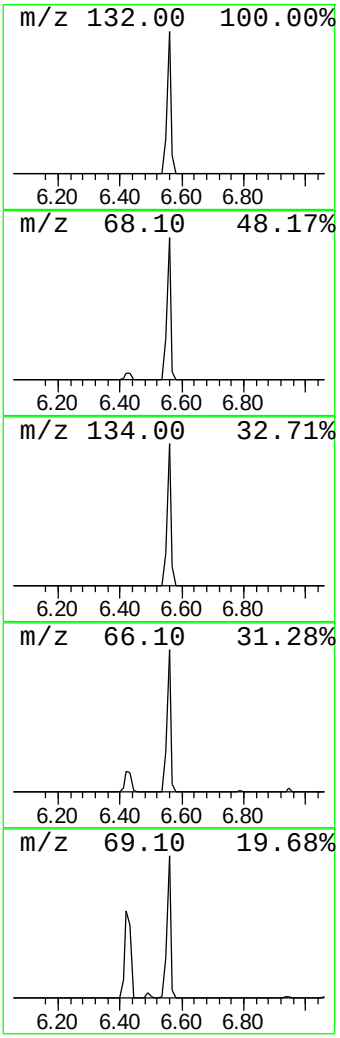
****

Peak Number 5 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	67.84 ng	2346950	1,4-Dichlorobenzene-d4	6.79

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	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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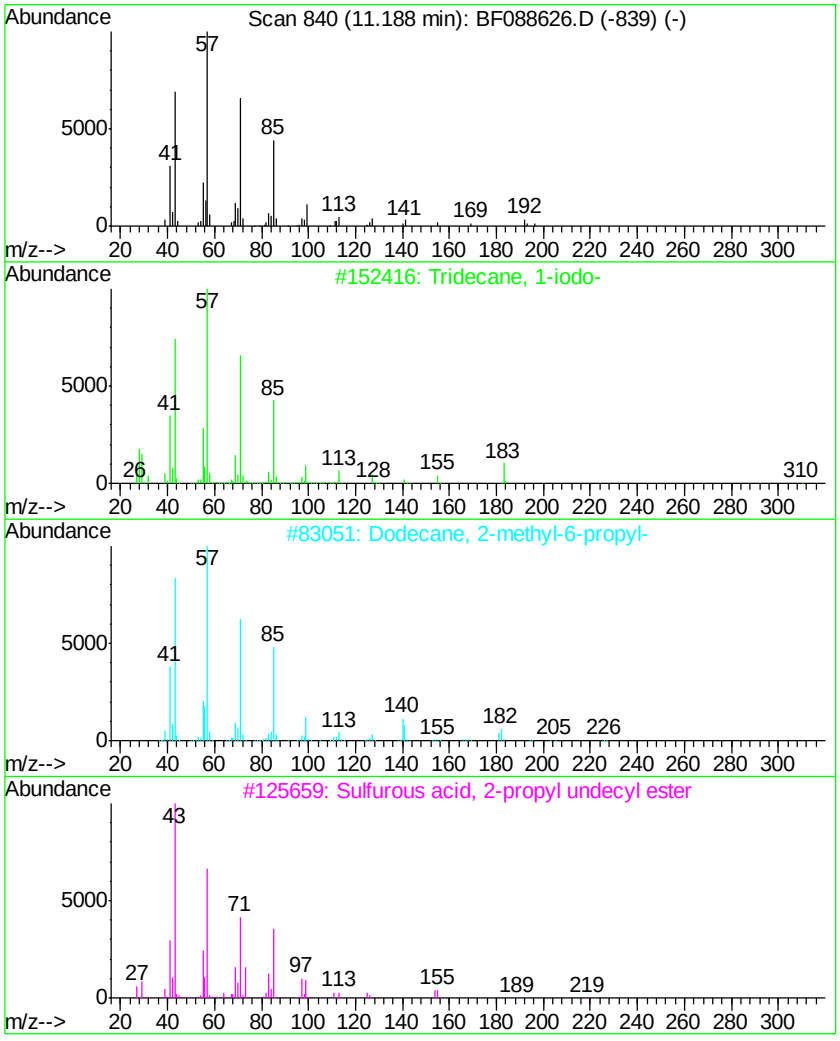
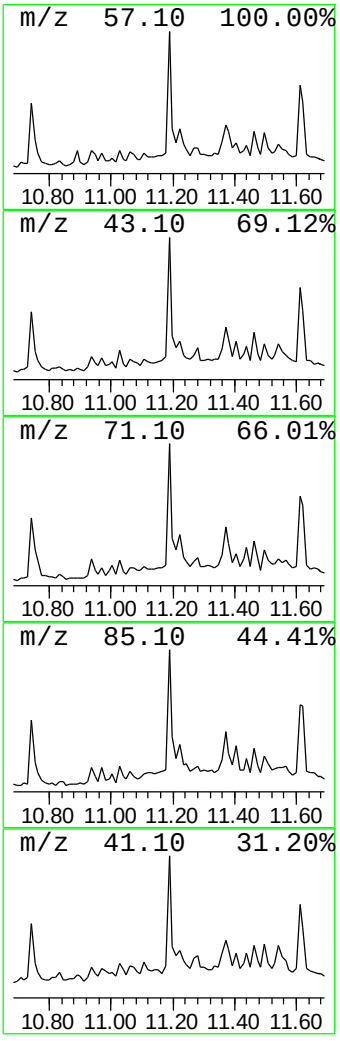
Peak Number 7 Tridecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.49 ng	103399	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	64
4	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	64
5	Heptacosane	380	C27H56	000593-49-7	64





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Operator : UM/SJ
Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(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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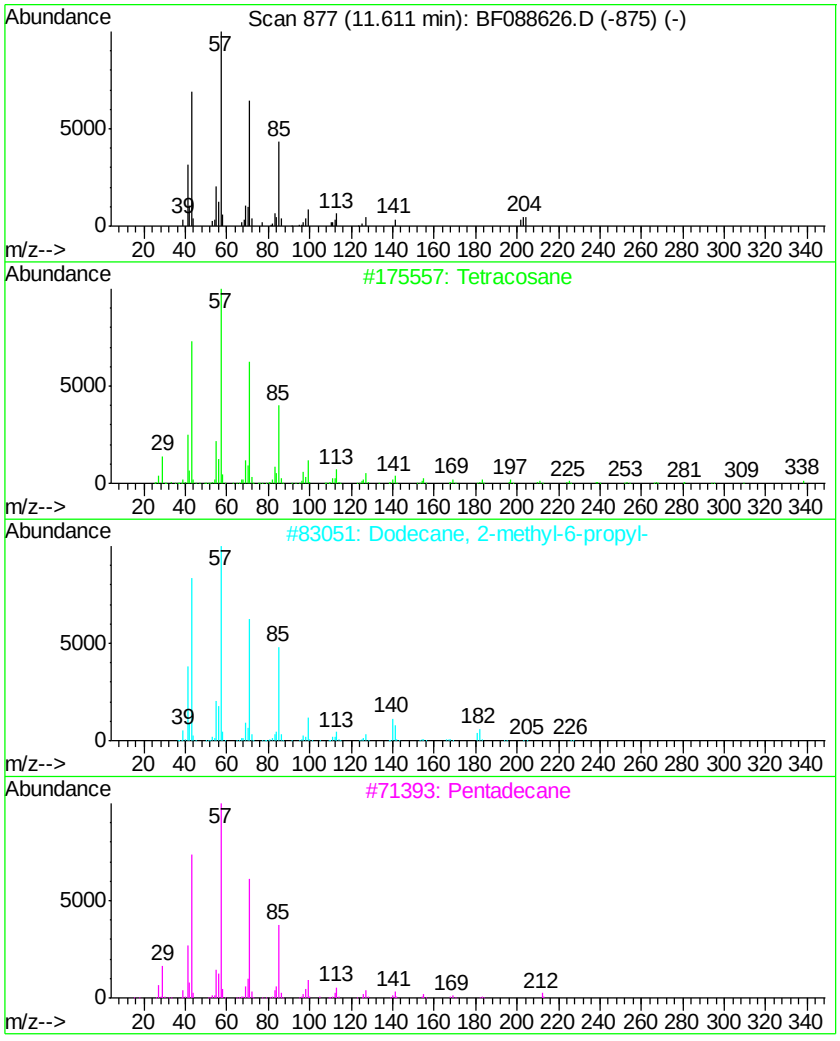
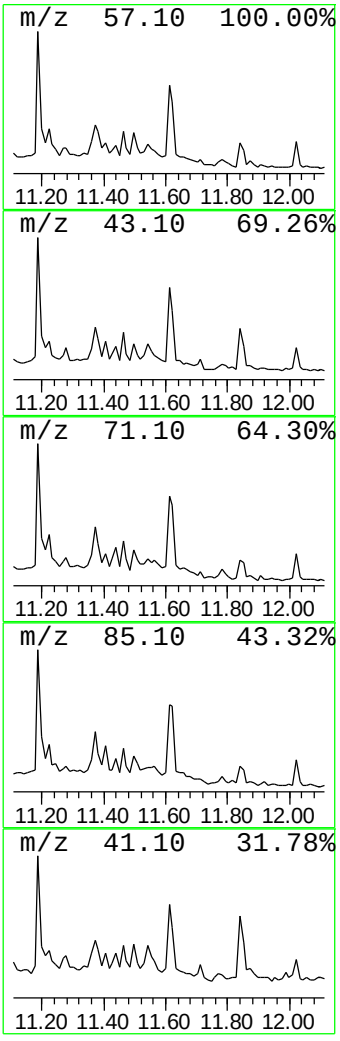
Peak Number 8 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	2.34 ng	97009	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	83
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Pentadecane	212	C15H32	000629-62-9	80
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5	Hexadecane	226	C16H34	000544-76-3	78





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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
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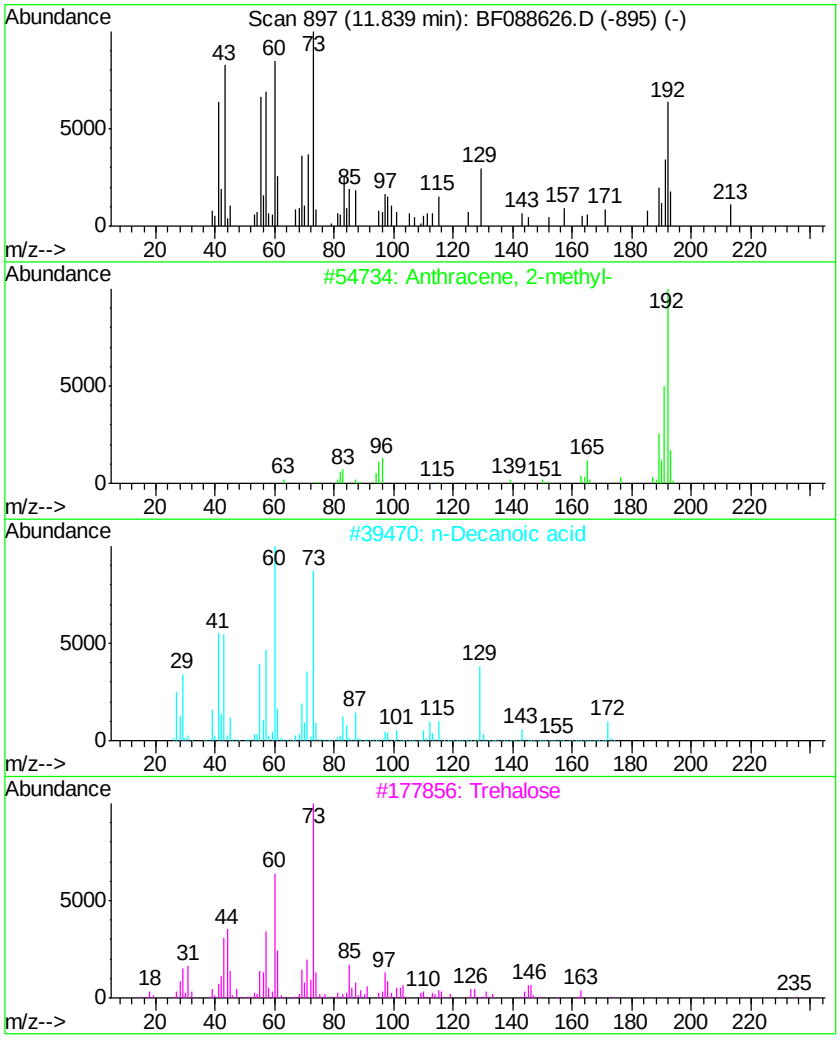
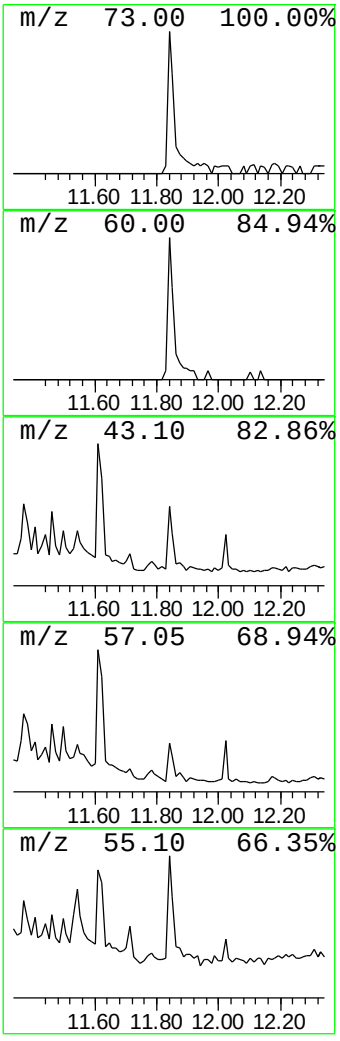
Peak Number 9 unknown11.84 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.14 ng	88935	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	43
2	n-Decanoic acid	172	C10H20O2	000334-48-5	38
3	Trehalose	342	C12H22O11	000099-20-7	35
4	Lactose	342	C12H22O11	000063-42-3	35
5	d-Lyxose	150	C5H10O5	001114-34-7	35





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Operator : UM/SJ
Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(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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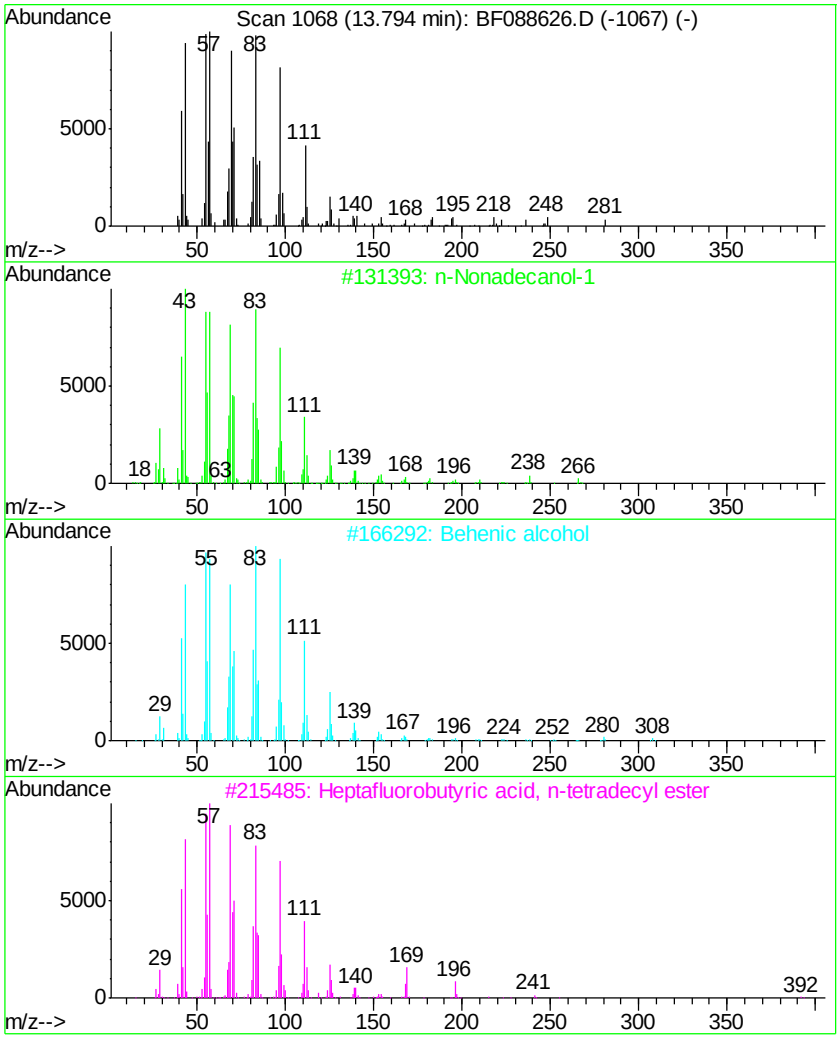
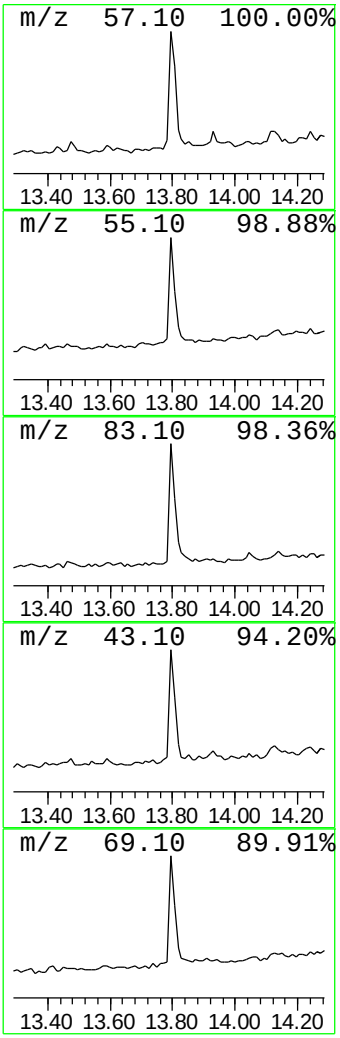
Peak Number 10 n-Nonadecanol-1 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	2.91 ng	143837	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	91





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Misc :
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Instrument : BNA_F
ClientSampleId : S4-B2(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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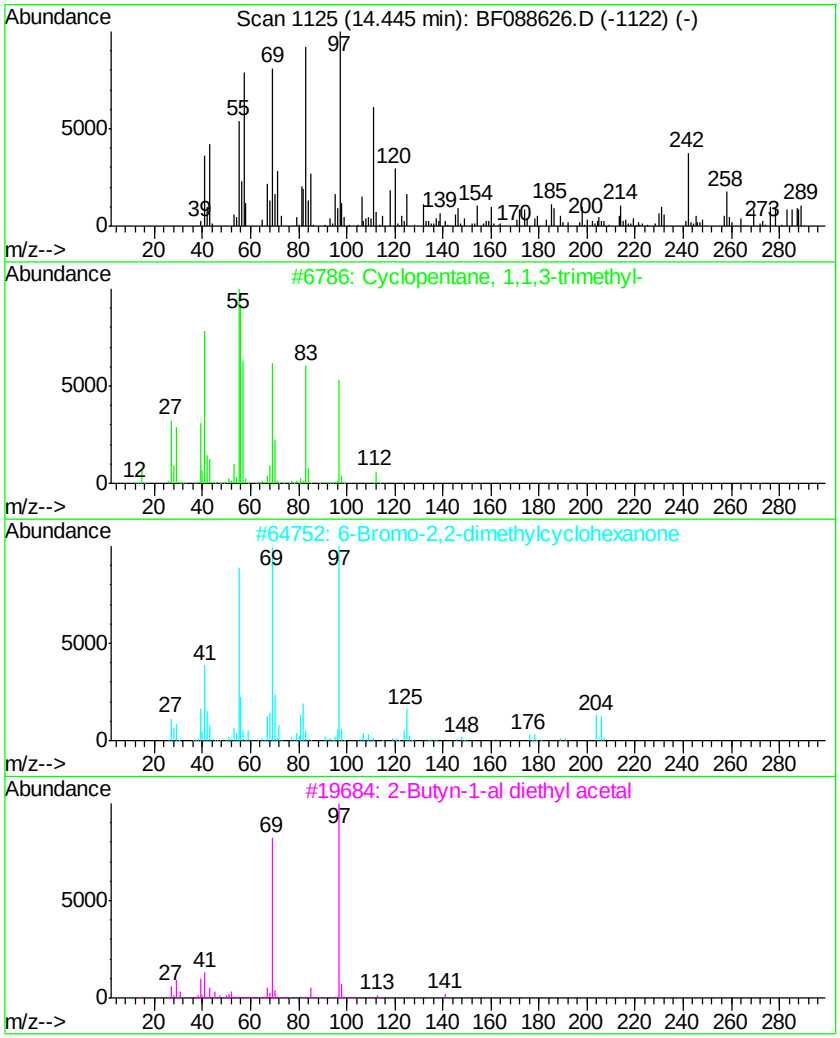
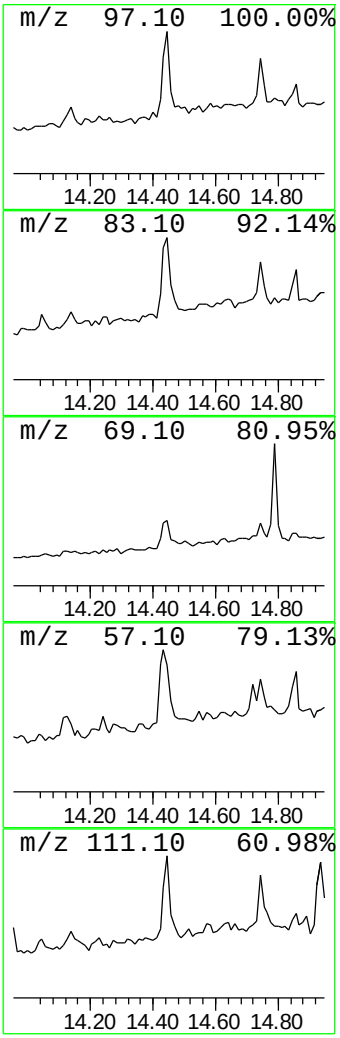
Peak Number 11 Cyclopentane, 1,1,3-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.06 ng	101858	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	52
2	6-Bromo-2,2-dimethylcyclohexanone	204	C8H13BrO	021690-26-6	38
3	2-Butyn-1-al diethyl acetal	142	C8H14O2	002806-97-5	35
4	Bicyclo[3.1.1]heptan-3-one, 2-et...	166	C11H18O	1000163-95-8	22
5	Cyclopentaneacetic acid, ethenyl...	154	C9H14O2	045955-66-6	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088626.D
Acq On : 2 Jul 2016 19:35
Operator : UM/SJ
Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(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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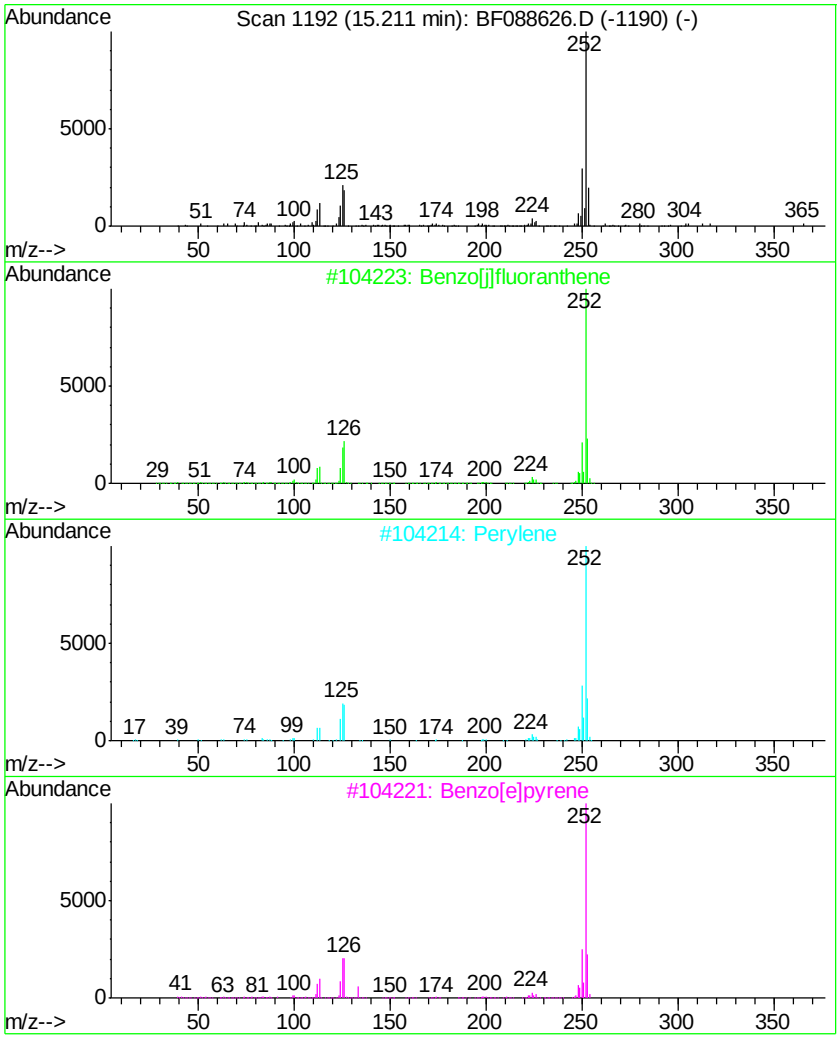
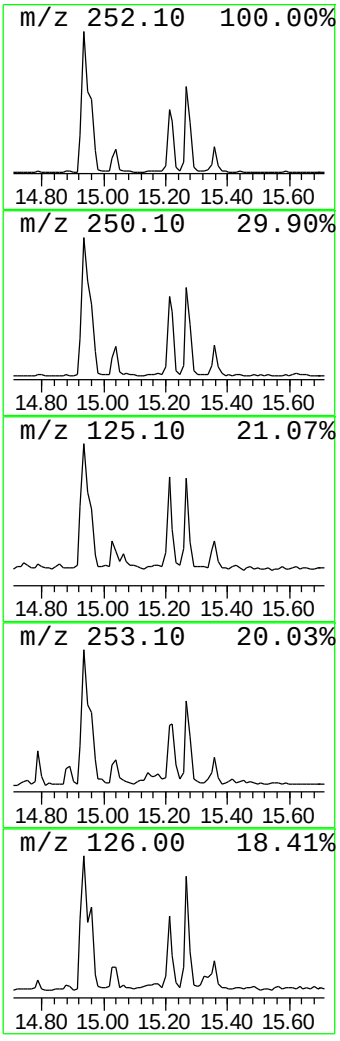
Peak Number 13 Benzo[j]fluoranthene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	4.20 ng	121709	Perylene-d12	15.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
2	Perylene	252	C20H12	000198-55-0	94
3	Benzo[e]pyrene	252	C20H12	000192-97-2	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070216\
Data File : BF088626.D
Acq On : 2 Jul 2016 19:35
Operator : UM/SJ
Sample : H3847-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S4-B2(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
unknown3.00	3.00	6.2	ng	214803	1	6.79	691912	20.0
2-Pentanone, 4-hy...	4.96	6.0	ng	206545	1	6.79	691912	20.0
unknown6.56	6.56	67.8	ng	2346950	1	6.79	691912	20.0
Tridecane, 1-iodo-	11.19	2.5	ng	103399	4	11.30	830075	20.0
Tetracosane	11.61	2.3	ng	97009	4	11.30	830075	20.0
unknown11.84	11.84	2.1	ng	88935	4	11.30	830075	20.0
n-Nonadecanol-1	13.79	2.9	ng	143837	5	13.93	989349	20.0
Cyclopentane, 1,1...	14.45	2.1	ng	101858	5	13.93	989349	20.0
Benzo[j]fluoranthene	15.21	4.2	ng	121709	6	15.34	579290	20.0