LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

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-BF072016.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	1.713	9	11	42	rVB	441487	894087	62.55%	7.100%
2	4.707	270	273	280	rBV	40233	64900	4.54%	0.515%
3	5.164	310	313	333	rBV	849474	1211130	84.72%	9.618%
4	6.239	404	407	414	rBV	993494	1300712	90.99%	10.330%
5	6.342	414	416	419	rBV	817123	1139354	79.70%	9.048%
6	6.582	435	437	448	rBV	203574	260899	18.25%	2.072%
7	6.730	448	450	453	rBV	934100	917838	64.21%	7.289%
8	7.153	484	487	504	rBV	596918	818759	57.28%	6.502%
9	7.862	547	549	560	rBV	419204	410164	28.69%	3.257%
10	8.948	641	644	646	rBV	1207192	1429488	100.00%	11.352%
11	9.336	676	678	681	rBV	109821	126747	8.87%	1.007%
12	9.611	699	702	704	rBV	384607	394823	27.62%	3.136%
13	10.399	768	771	773	rBV2	431318	640736	44.82%	5.088%
14	10.525	781	782	788	rVB2	17594	23382	1.64%	0.186%
15	10.971	819	821	823	rBV	19081	19882	1.39%	0.158%
16	11.085	828	831	836	rVV2	266717	368942	25.81%	2.930%
17	11.691	882	884	889	rVB2	14539	21802	1.53%	0.173%
18	12.285	934	936	940	rBV	103421	101347	7.09%	0.805%
19	12.502	953	955	958	rBV	170071	193666	13.55%	1.538%
20	12.582	958	962	964	rVB2	20956	23886	1.67%	0.190%
21	12.662	967	969	972	rBV	875303	873228	61.09%	6.935%
22	12.845	980	985	988	rVB	7296	16744	1.17%	0.133%
23	13.211	1014	1017	1019	rBV	59675	61526	4.30%	0.489%
24	13.257	1019	1021	1024	rVB2	10033	17769	1.24%	0.141%
25	13.577	1046	1049	1057	rBV2	43189	87916	6.15%	0.698%
26	13.702	1057	1060	1067	rVV2	277361	376570	26.34%	2.991%
27	13.897	1074	1077	1084	rVB2	13367	17841	1.25%	0.142%
28	14.091	1089	1094	1096	rBV	9481	16703	1.17%	0.133%
29	14.194	1099	1103	1110	rBV4	11951	38596	2.70%	0.307%
30	14.491	1125	1129	1131	rBV2	17959	25062	1.75%	0.199%
31	14.685	1144	1146	1152	rBV	44211	95273	6.66%	0.757%
32	14.777	1152	1154	1156	rVV	34483	37343	2.61%	0.297%
33	14.811	1156	1157	1164	rVB4	10060	22573	1.58%	0.179%
34	14.937	1166	1168	1171	rVV	25506	33370	2.33%	0.265%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

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-BF072016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.994	1171	1173	1175	rVV	33157	41417	2.90%	0.329%
36	15.040	1175	1177	1180	rVV	168257	260115	18.20%	2.066%
37	15.097	1180	1182	1185	rVB2	16366	25263	1.77%	0.201%
38	15.451	1210	1213	1216	rBV	28359	36708	2.57%	0.292%
39	15.863	1247	1249	1255	rVB3	10172	22442	1.57%	0.178%
40	16.263	1281	1284	1288	rVB2	13610	25306	1.77%	0.201%
41	16.343	1288	1291	1293	rBV	8653	18783	1.31%	0.149%
42	16.628	1312	1316	1321	rBV	8604	23036	1.61%	0.183%
43	16.743	1323	1326	1332	rVV6	6909	25119	1.76%	0.199%
44	16.903	1336	1340	1343	rVB2	5064	14895	1.04%	0.118%
45	18.377	1462	1469	1472	rBV6	4322	15840	1.11%	0.126%

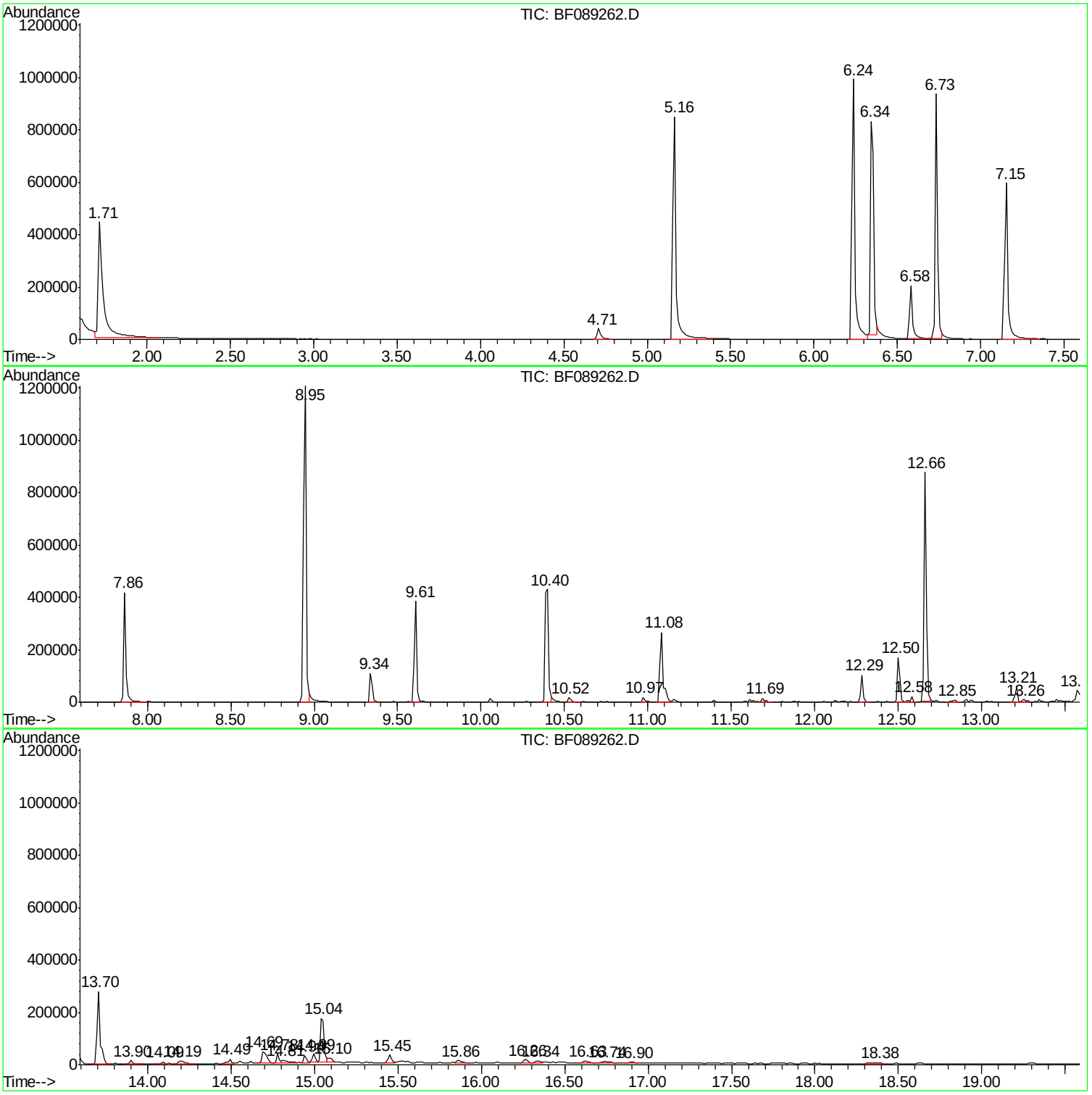
Sum of corrected areas: 12591982

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

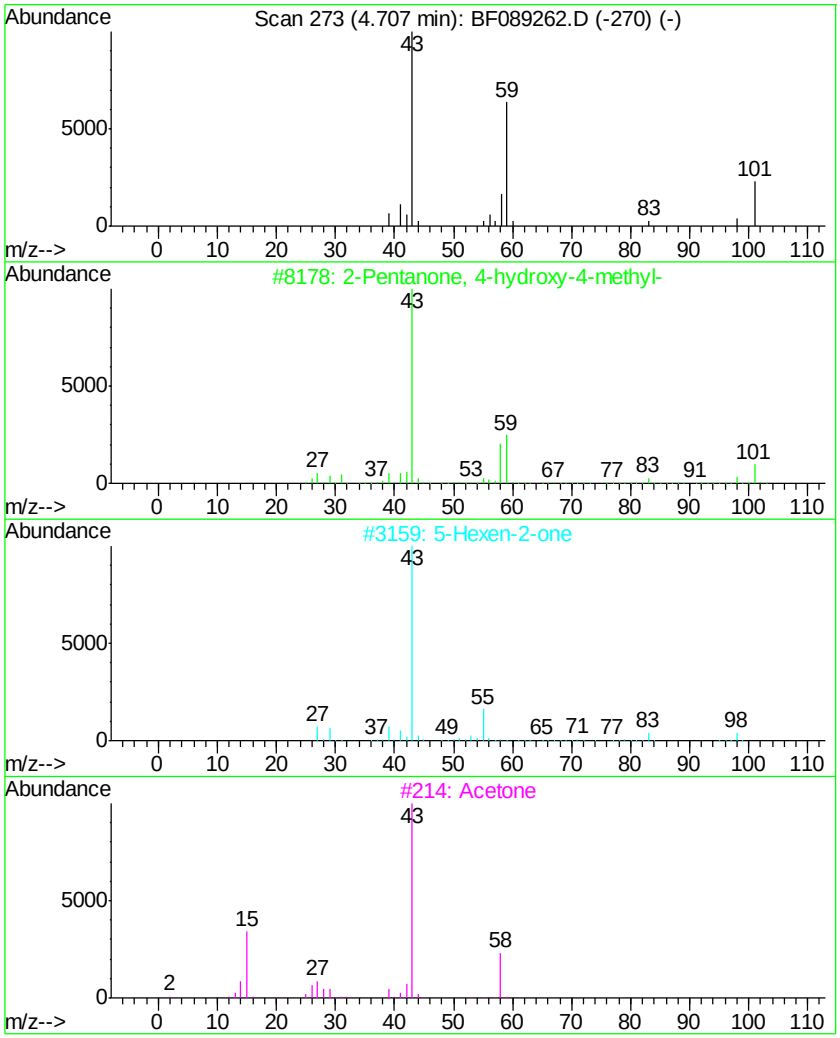
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

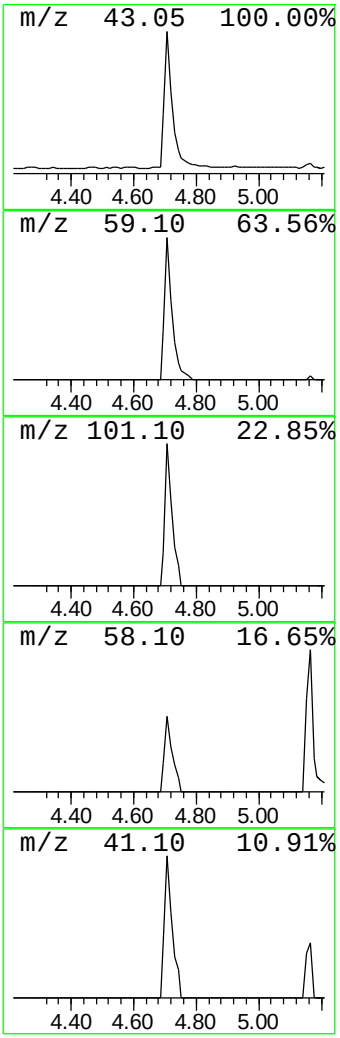
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	4.98 ng	64900	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Acetone	58	C3H6O	000067-64-1	9
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

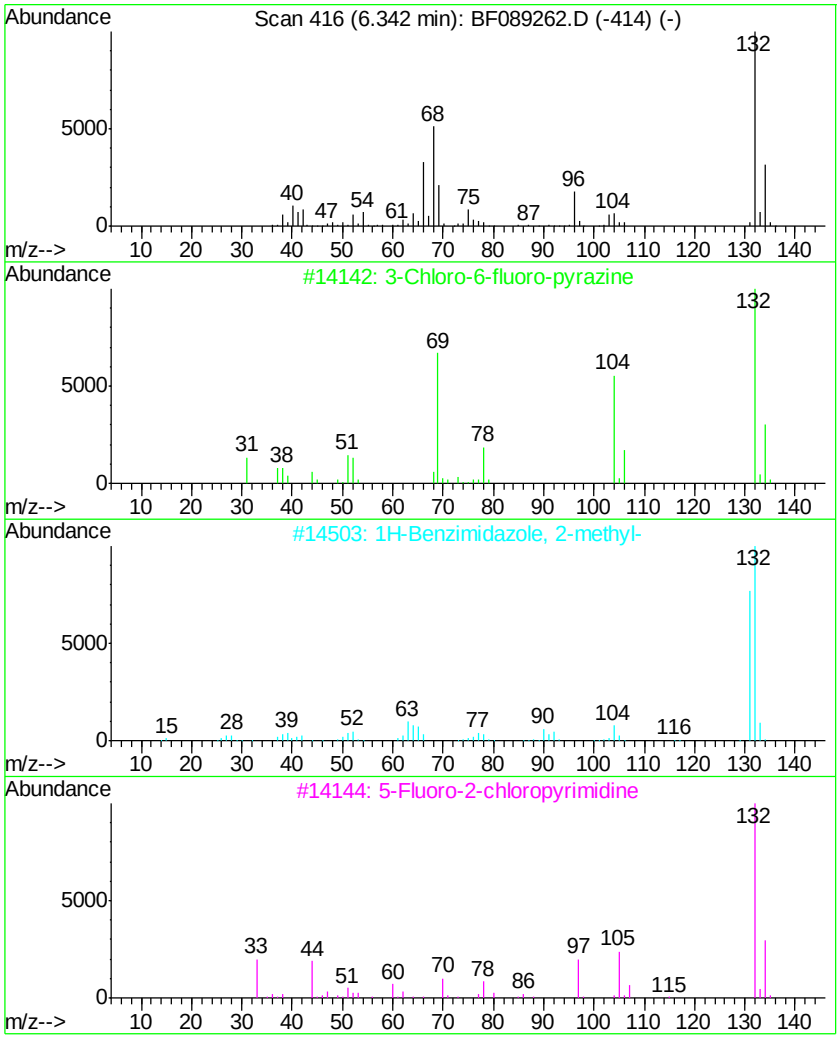
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

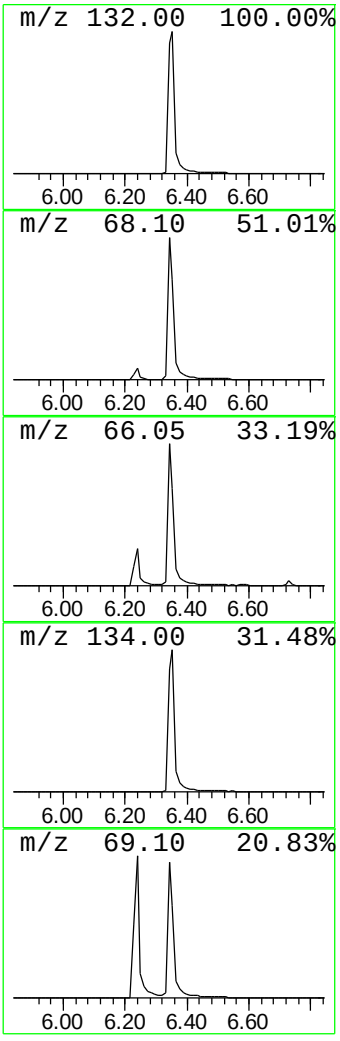
****

Peak Number 3 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	87.34 ng	1139350	1,4-Dichlorobenzene-d4	6.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

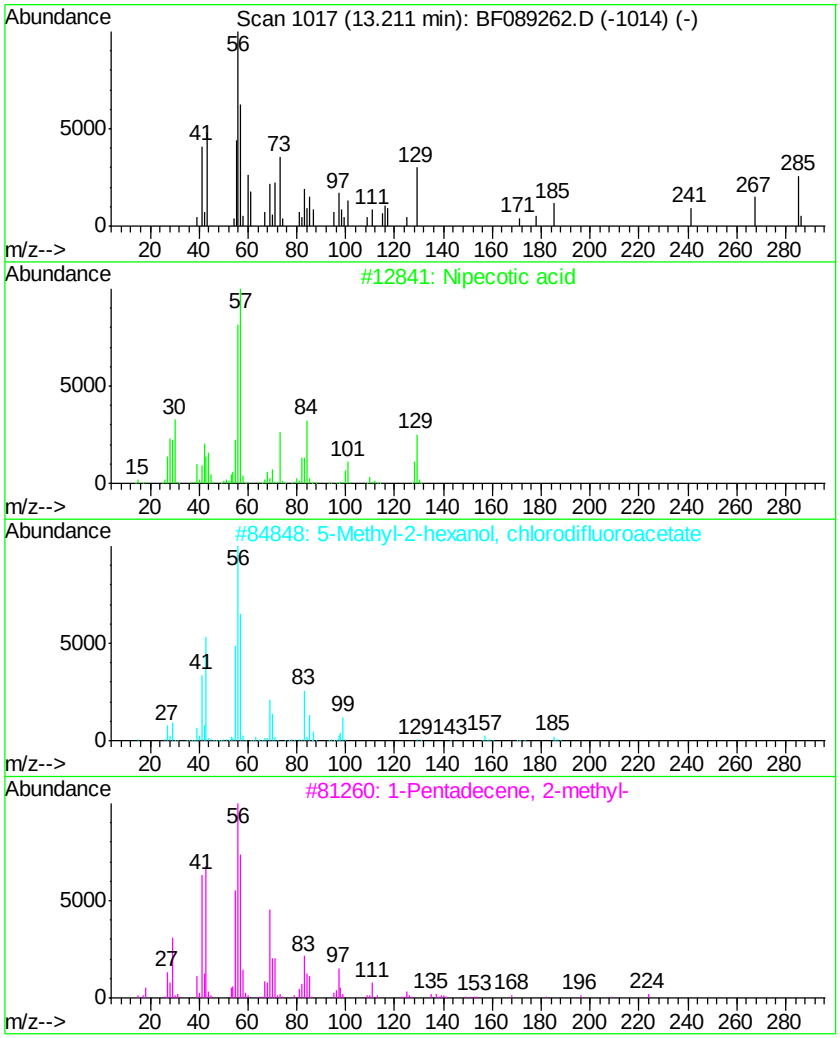
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

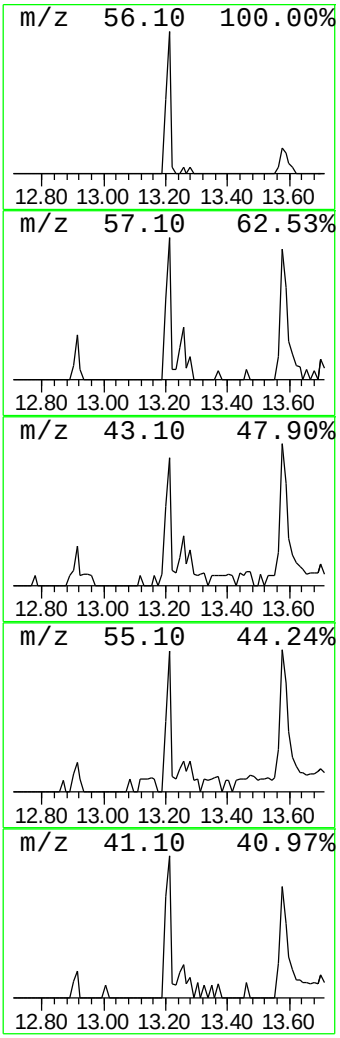
****

Peak Number 5 unknown13.21 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.21	3.27 ng	61526	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nipecotic acid	129	C6H11NO2	000498-95-3	37
2	5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1000376-27-1	27
3	1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	27
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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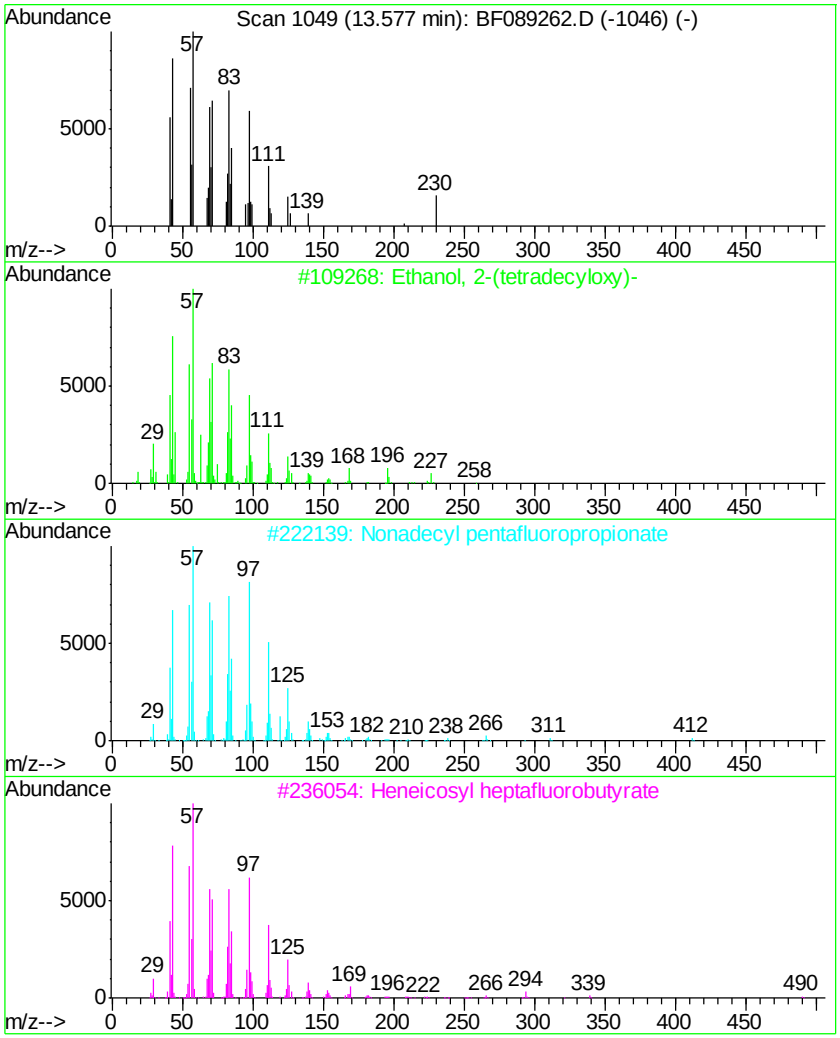
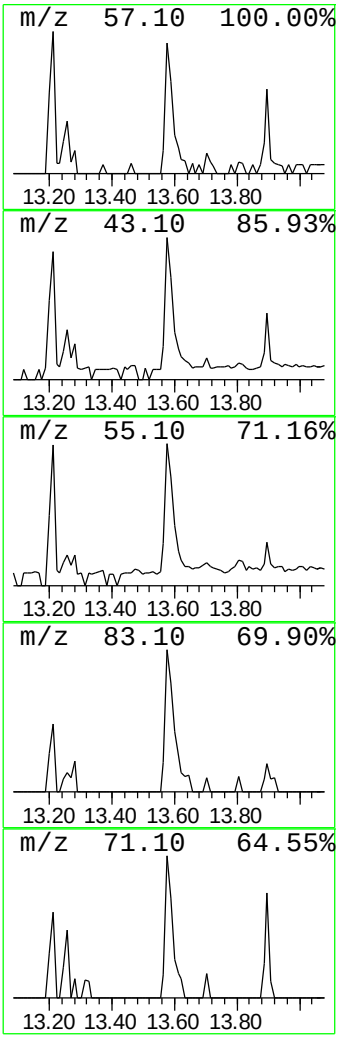
Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.58	4.67 ng	87916	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	76





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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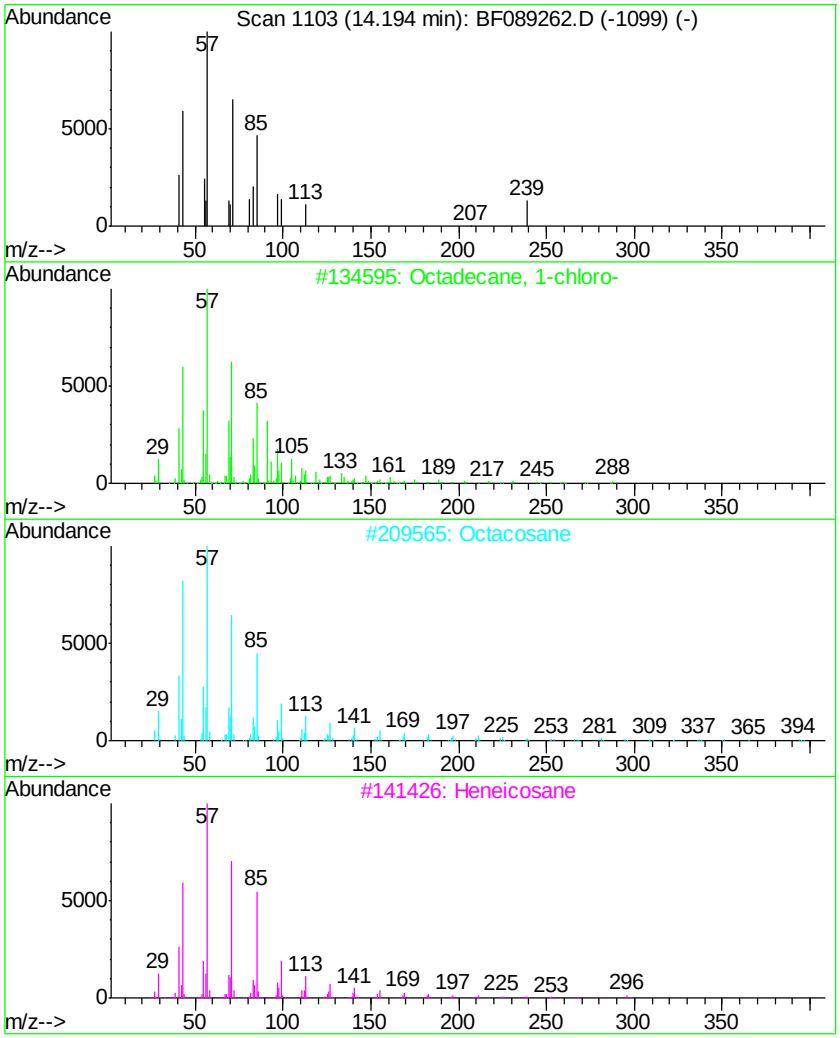
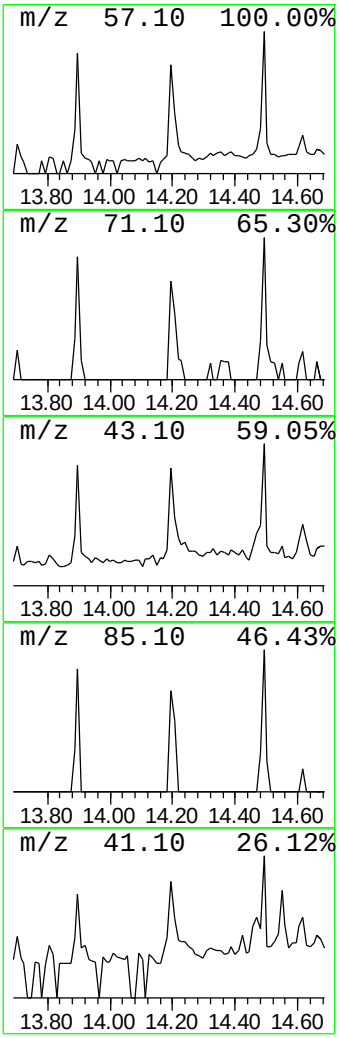
Peak Number 7 Octadecane, 1-chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.05 ng	38596	Chrysene-d12	13.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
2	Octacosane	394	C28H58	000630-02-4	64
3	Heneicosane	296	C21H44	000629-94-7	59
4	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	59
5	Hexadecane	226	C16H34	000544-76-3	59





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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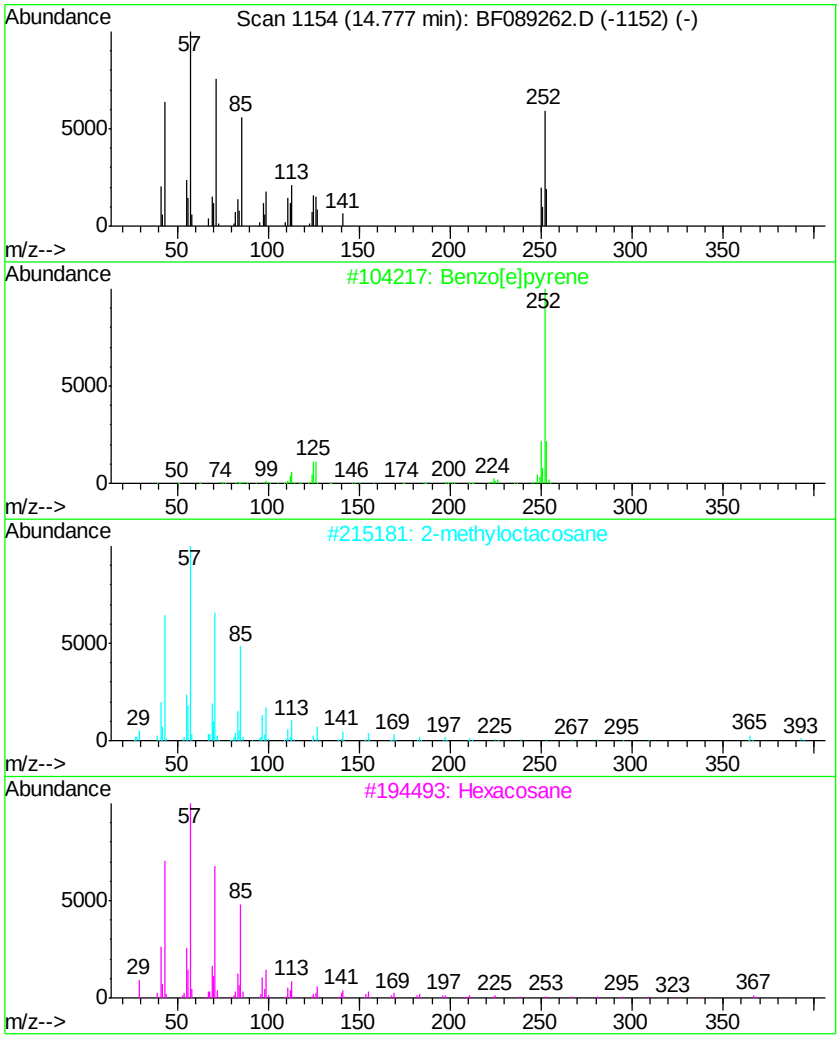
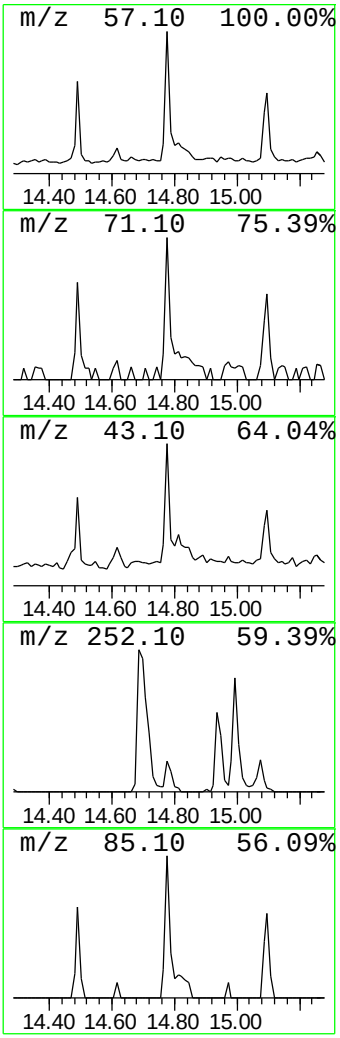
Peak Number 8 unknown14.78 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	2.87 ng	37343	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	49
2	2-methyloctacosane	408	C29H60	1000376-72-8	43
3	Hexacosane	366	C26H54	000630-01-3	43
4	Octacosane	394	C28H58	000630-02-4	43
5	Pentacosane	352	C25H52	000629-99-2	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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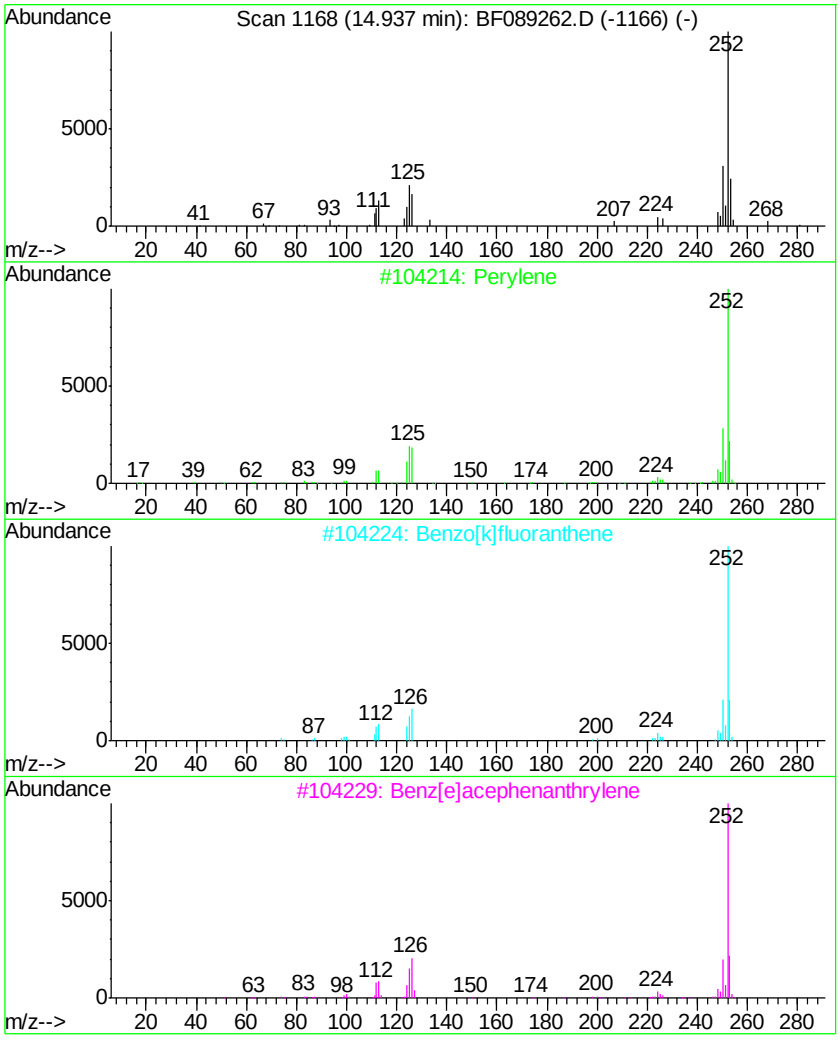
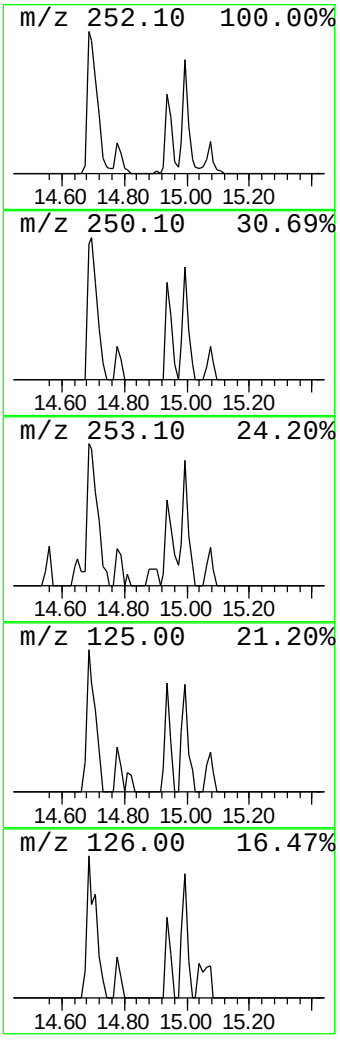
Peak Number 9 Perylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.57 ng	33370	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	95
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Benzo[e]pyrene	252	C20H12	000192-97-2	81





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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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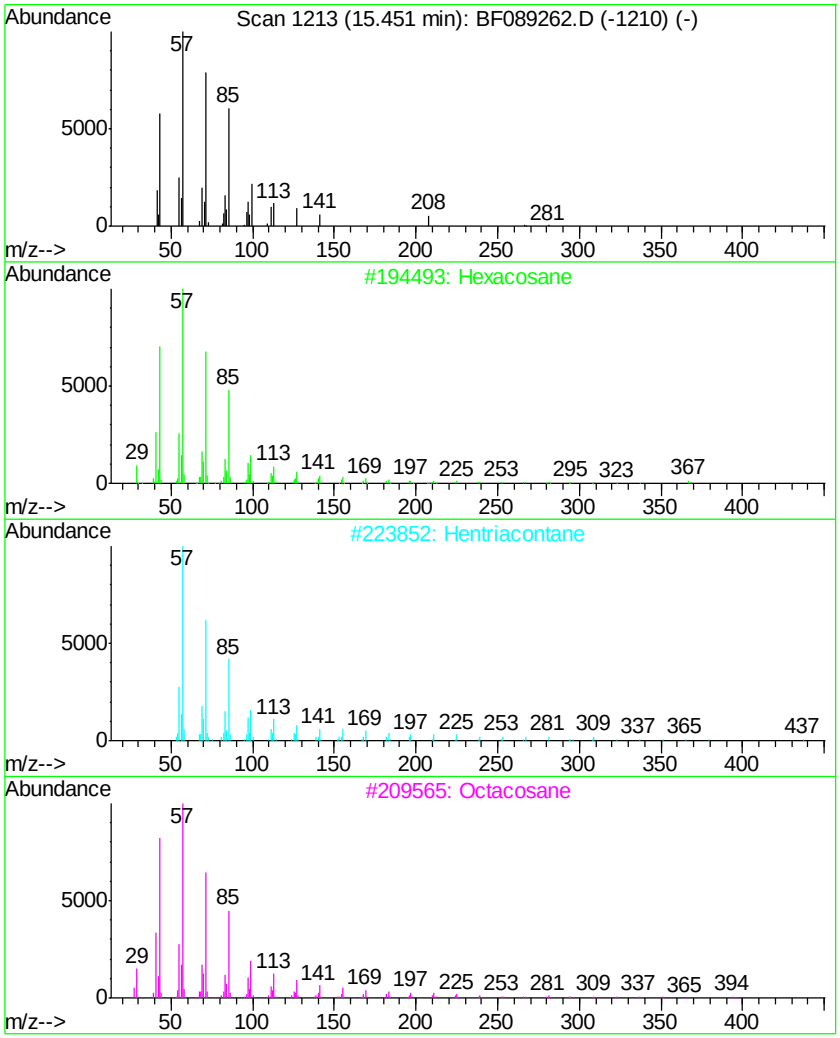
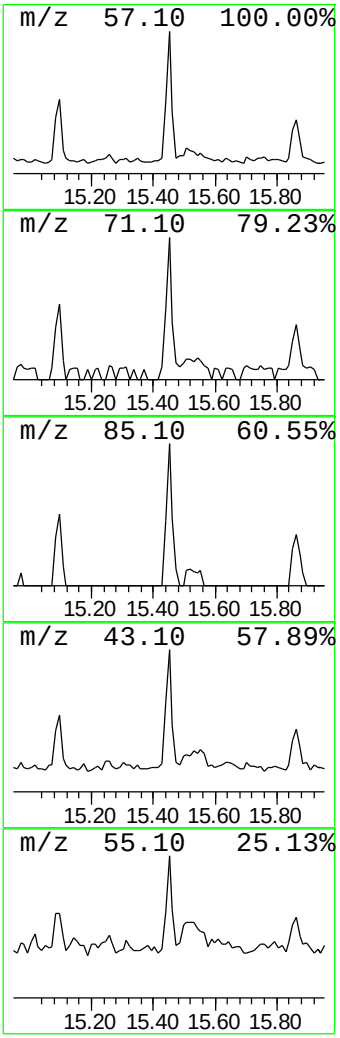
Peak Number 10 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.82 ng	36708	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072316\
Data File : BF089262.D
Acq On : 24 Jul 2016 6:05
Operator : UM/SJ
Sample : H4151-06
Misc :
ALS Vial : 60 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-07-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.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...	4.71	5.0	ng	64900	1	6.58	260899	20.0
unknown6.34	6.34	87.3	ng	1139350	1	6.58	260899	20.0
unknown13.21	13.21	3.3	ng	61526	5	13.70	376570	20.0
Ethanol, 2-(tetra...	13.58	4.7	ng	87916	5	13.70	376570	20.0
Octadecane, 1-chl...	14.19	2.0	ng	38596	5	13.70	376570	20.0
unknown14.78	14.78	2.9	ng	37343	6	15.05	260115	20.0
Perylene	14.94	2.6	ng	33370	6	15.05	260115	20.0
Hexacosane	15.45	2.8	ng	36708	6	15.05	260115	20.0