LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

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-BF012417.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	3.447	117	119	131	rBV	22115	89030	1.45%	0.167%
2	4.841	239	241	247	rBV	34679	67883	1.11%	0.127%
3	5.173	267	270	281	rBV	1807630	2878816	46.92%	5.405%
4	5.596	304	307	309	rBV	4746538	5381538	87.70%	10.104%
5	6.624	394	397	400	rBV	4409785	5992132	97.65%	11.250%
6	6.750	405	408	410	rBV	5247069	5693341	92.78%	10.689%
7	6.967	425	427	430	rBV	1084700	1138497	18.55%	2.137%
8	7.127	438	441	444	rBV	3591370	4299724	70.07%	8.073%
9	7.539	474	477	480	rBV	2655519	4165172	67.88%	7.820%
10	7.630	482	485	487	rVV	60873	70642	1.15%	0.133%
11	8.259	538	540	543	rBV	1170139	1500799	24.46%	2.818%
12	9.356	632	636	638	rBV	4423184	6136232	100.00%	11.521%
13	9.745	668	670	672	rBV	1197127	1012316	16.50%	1.901%
14	9.950	686	688	691	rBV2	50902	81594	1.33%	0.153%
15	10.031	692	695	697	rBV	1937241	1650252	26.89%	3.098%
16	10.453	728	732	734	rVB2	123686	191590	3.12%	0.360%
17	10.682	748	752	755	rBV	45252	83719	1.36%	0.157%
18	10.831	762	765	767	rBV	2596660	3267965	53.26%	6.136%
19	10.933	772	774	778	rVB	155830	220256	3.59%	0.414%
20	11.231	798	800	803	rBV2	86194	125327	2.04%	0.235%
21	11.379	811	813	814	rBV	198217	160664	2.62%	0.302%
22	11.413	814	816	819	rVB	56246	70901	1.16%	0.133%
23	11.516	823	825	828	rBV	1339503	1569438	25.58%	2.947%
24	11.802	848	850	852	rBV	115208	144782	2.36%	0.272%
25	12.214	884	886	888	rBV	102106	92248	1.50%	0.173%
26	12.739	930	932	934	rBV	79192	85631	1.40%	0.161%
27	12.968	949	952	954	rBV	65382	80196	1.31%	0.151%
28	13.117	962	965	967	rBV	4053013	4385621	71.47%	8.234%
29	14.008	1041	1043	1049	rVB	105444	154750	2.52%	0.291%
30	14.168	1054	1057	1059	rVV	966563	1076776	17.55%	2.022%
31	14.625	1095	1097	1099	rBV2	49217	61612	1.00%	0.116%
32	15.654	1184	1187	1191	rVB	751103	1039430	16.94%	1.951%
33	16.363	1247	1249	1255	rVB2	66794	143301	2.34%	0.269%
34	16.808	1286	1288	1294	rVB	68319	150988	2.46%	0.283%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHA-SB-03-2-4

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-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

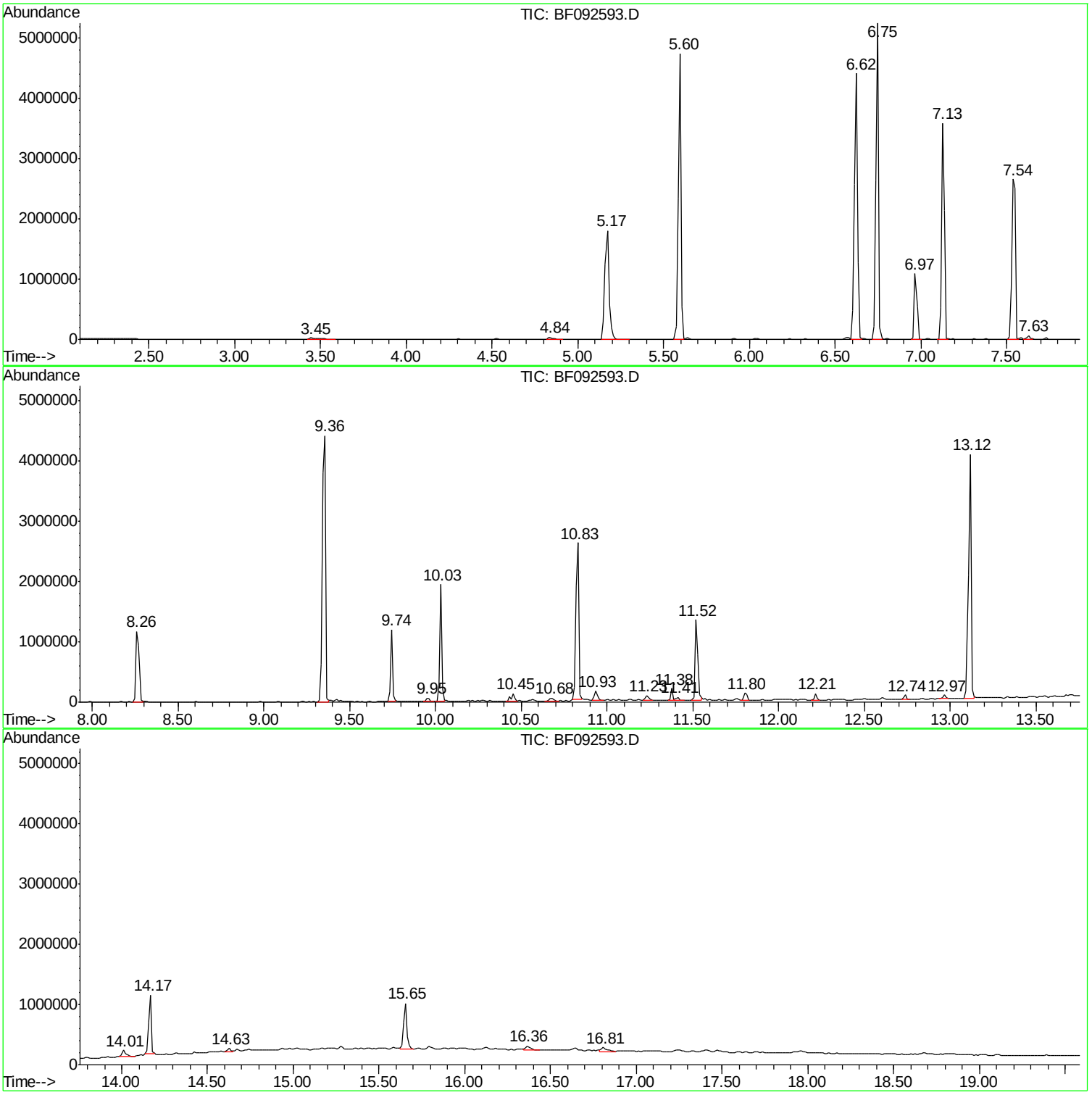
Sum of corrected areas: 53263163

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
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Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

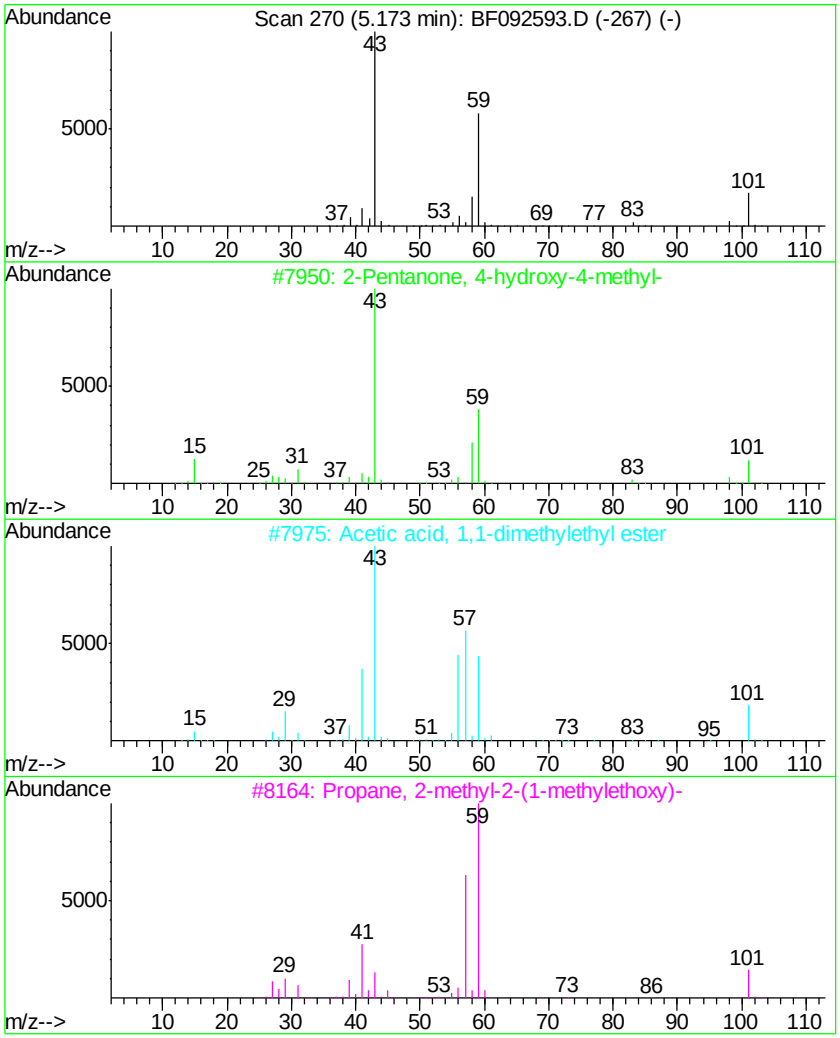
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

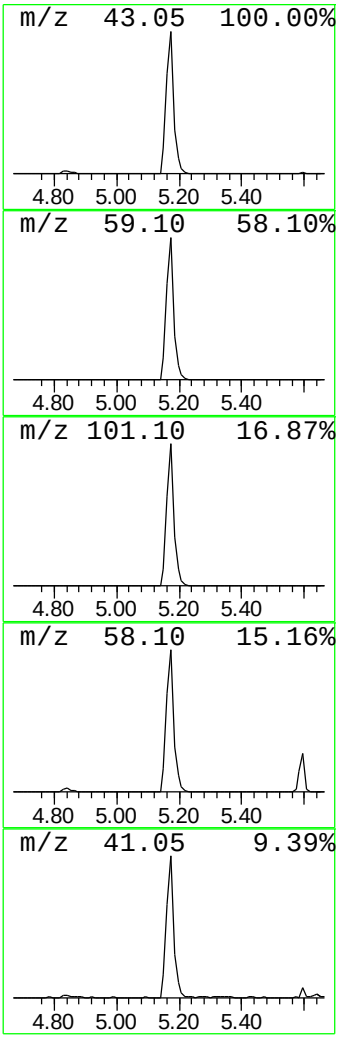
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	50.57 ng	2878820	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

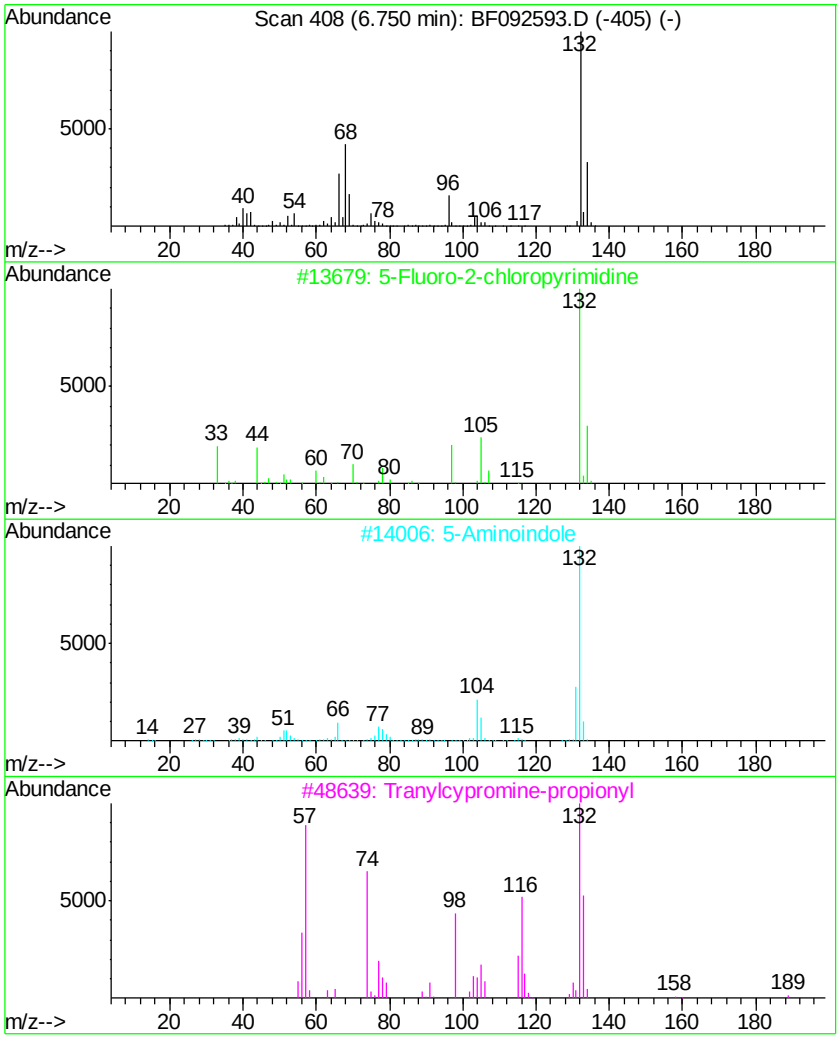
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

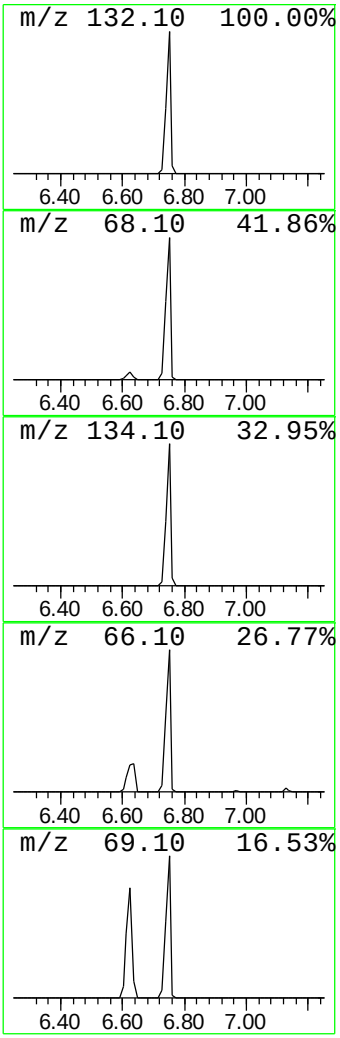
****

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	100.02 ng	5693340	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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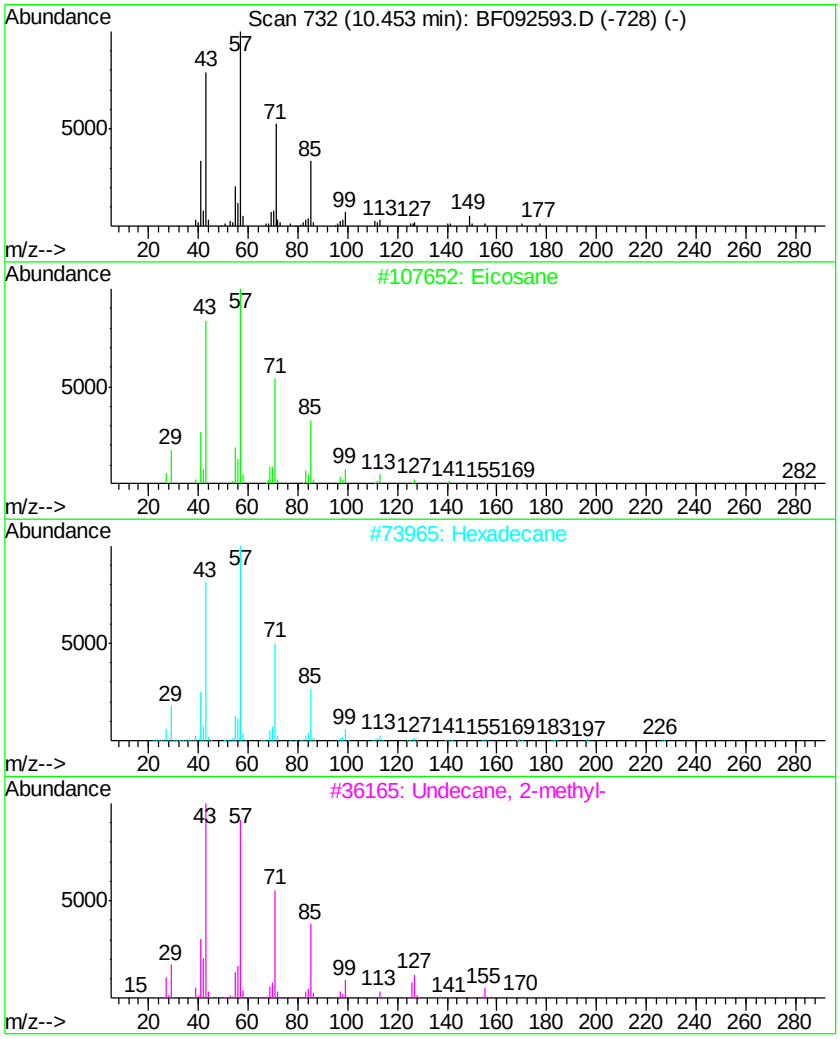
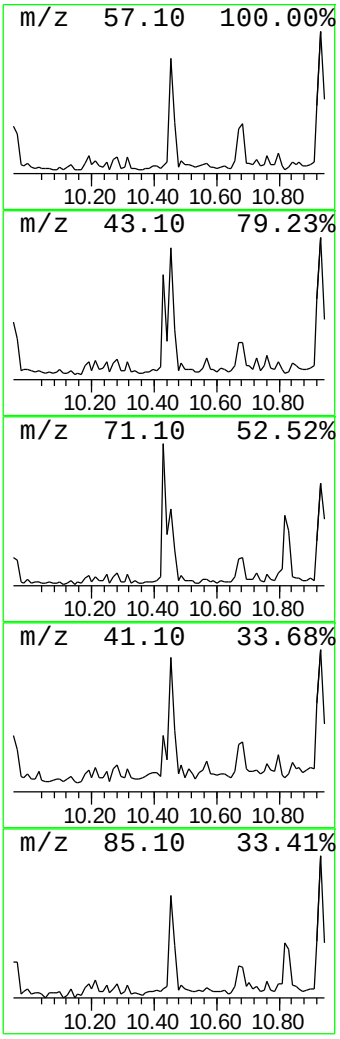
Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.45	2.32 ng	191590	Acenaphthene-d10	10.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Hexadecane	226	C16H34	000544-76-3	87
3	Undecane, 2-methyl-	170	C12H26	007045-71-8	80
4	Undecane, 5-methyl-	170	C12H26	001632-70-8	74
5	Undecane, 4-methyl-	170	C12H26	002980-69-0	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

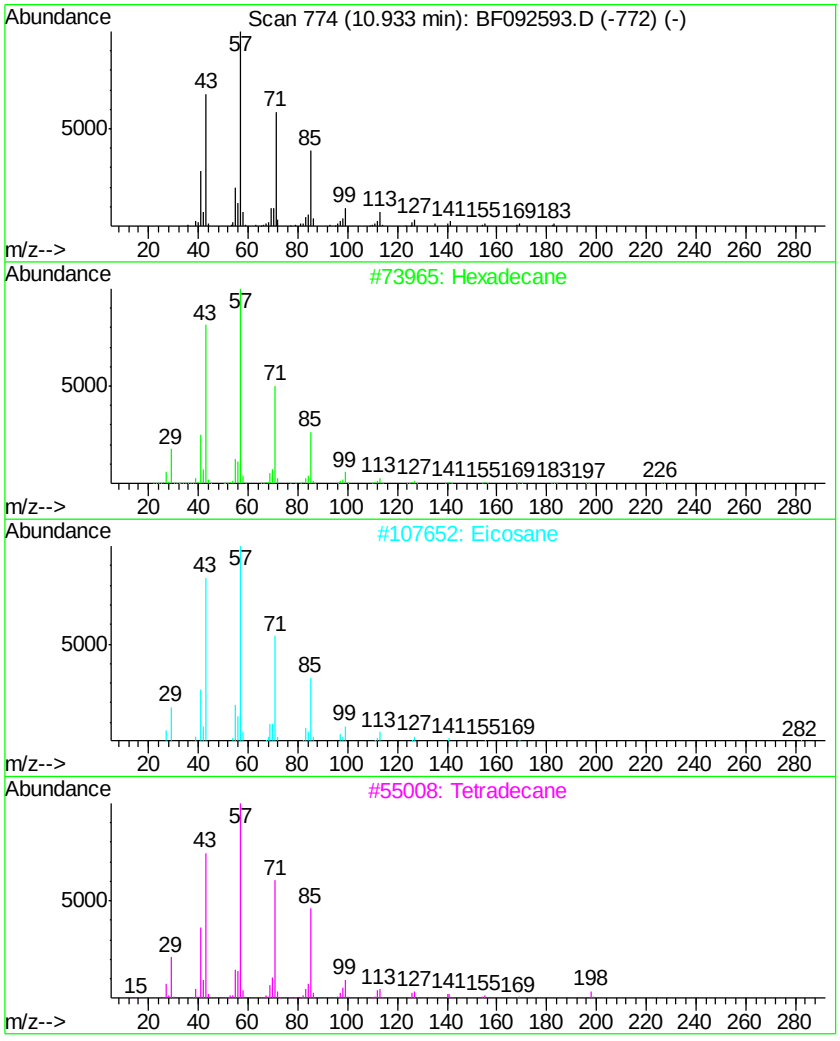
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

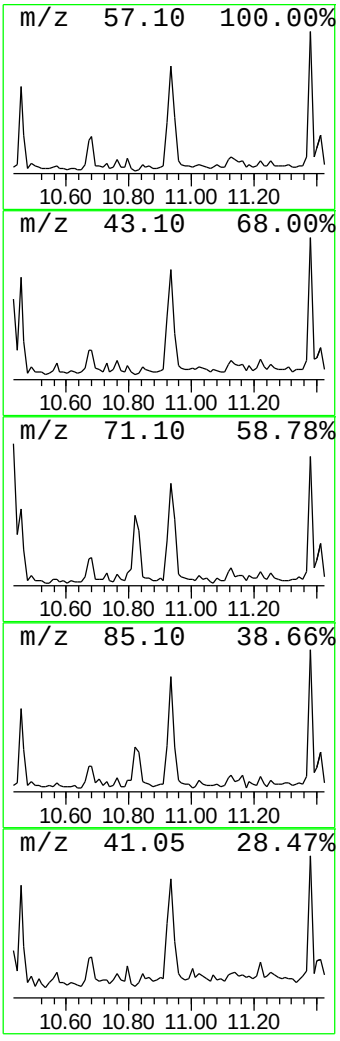
****

Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	2.81 ng	220256	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Eicosane	282	C20H42	000112-95-8	90
3	Tetradecane	198	C14H30	000629-59-4	87
4	Tetracosane	338	C24H50	000646-31-1	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

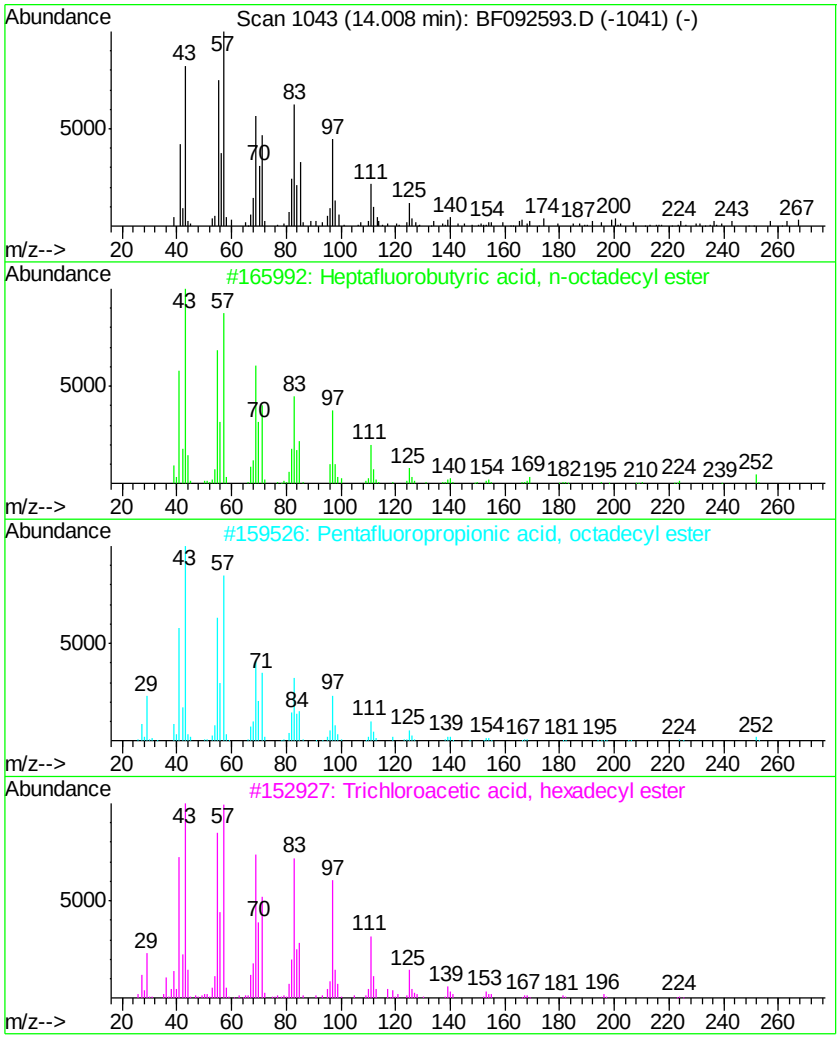
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

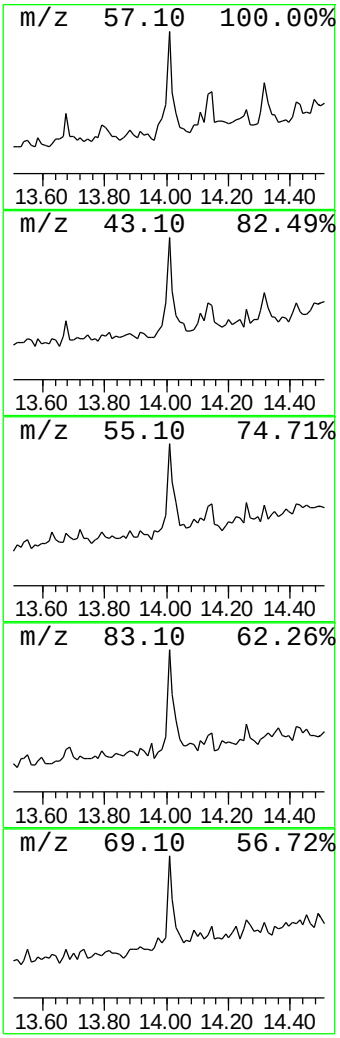
****

Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	2.87 ng	154750	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

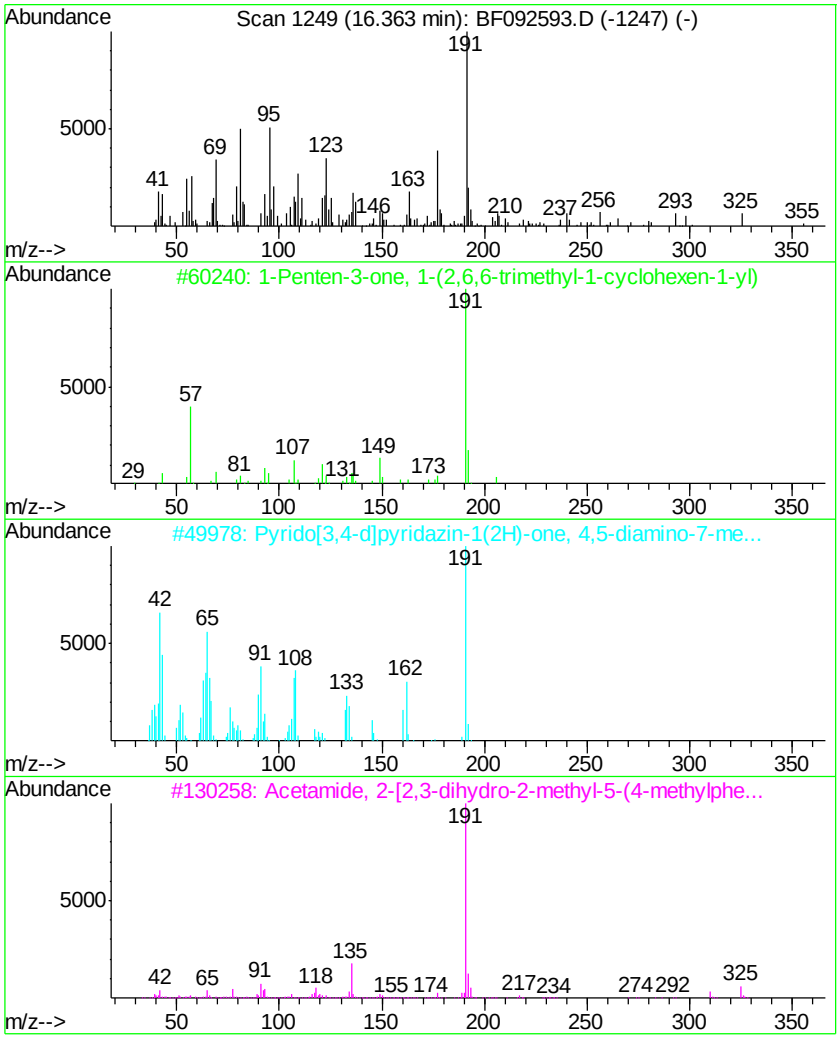
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

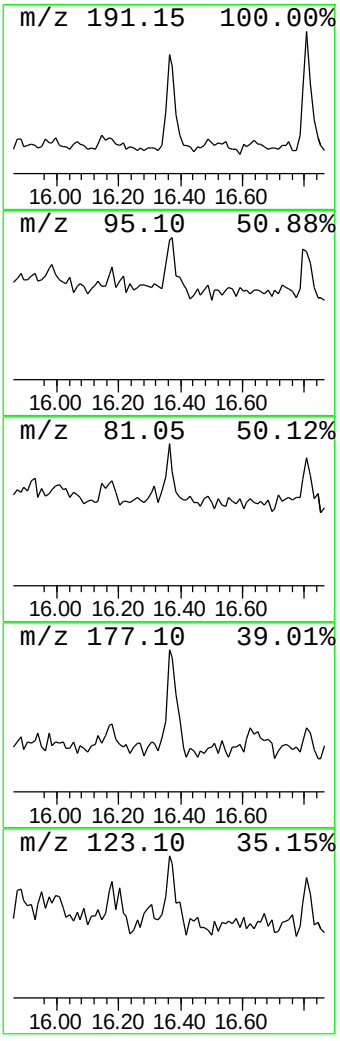
****

Peak Number 8 unknown16.36 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	2.76 ng	143301	Perylene-d12	15.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	46
2	Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	35
3	Acetamide, 2-[2,3-dihydro-2-meth...	325	C18H19N3OS	1000276-37-8	27
4	2-Amino-4-methyl-6-(2-thienyl)py...	191	C9H9N3S	026963-43-9	27
5	3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	27





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHA-SB-03-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

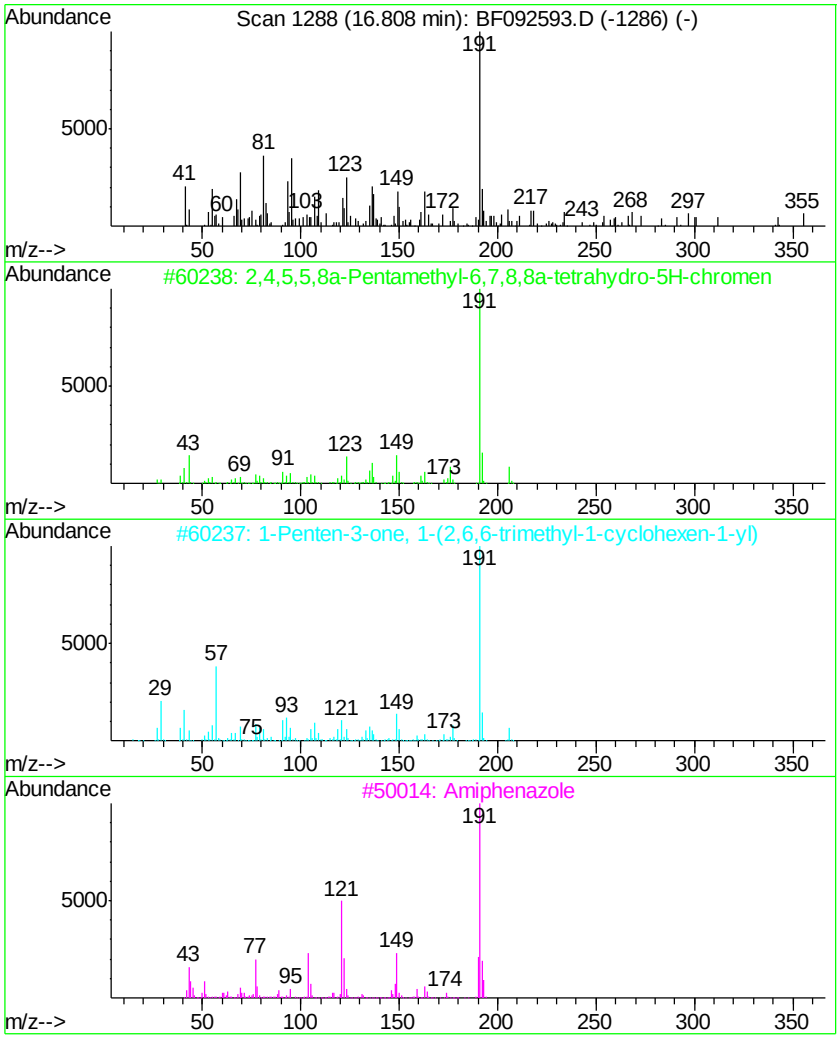
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

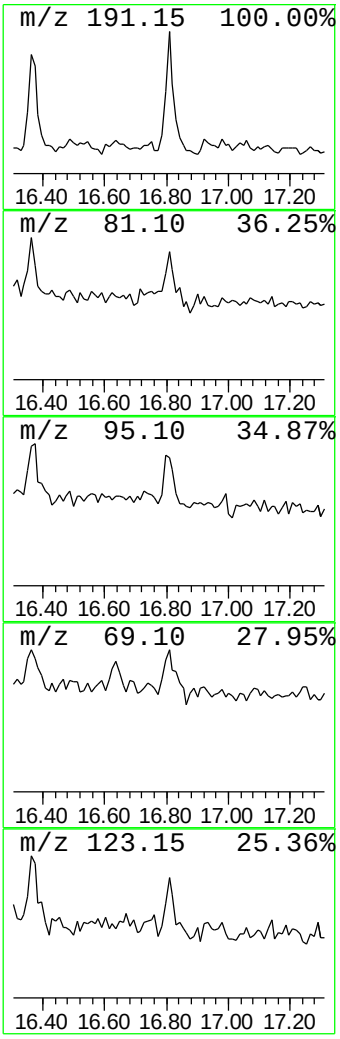
****

Peak Number 9 2,4,5,5,8a-Pentamethyl-6,7,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.81	2.91 ng	150988	Perylene-d12	15.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	59
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	49
3	Amiphenazole	191	C9H9N3S	000490-55-1	47
4	Cyclopropene-3-carbohydrazide, 1...	371	C22H17N3O3	1000259-44-9	43
5	Anthracene, 9-butyl-	234	C18H18	001498-69-7	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012717\
Data File : BF092593.D
Acq On : 27 Jan 2017 23:16
Operator : SJ/MA
Sample : I1448-07
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.17	50.6	ng	2878820	1	6.97	1138500	20.0
unknown6.75	6.75	100.0	ng	5693340	1	6.97	1138500	20.0
Eicosane	10.45	2.3	ng	191590	3	10.03	1650250	20.0
Hexadecane	10.93	2.8	ng	220256	4	11.52	1569440	20.0
Heptafluorobutyri...	14.01	2.9	ng	154750	5	14.17	1076780	20.0
unknown16.36	16.36	2.8	ng	143301	6	15.65	1039430	20.0
2,4,5,5,8a-Pentam...	16.81	2.9	ng	150988	6	15.65	1039430	20.0