LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-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-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	4.633	246	249	263	rBV	1073905	1941976	30.52%	3.832%
2	5.113	288	291	293	rBV	3411239	4280782	67.28%	8.447%
3	6.187	383	385	388	rBV	3465652	4645957	73.01%	9.167%
4	6.290	392	394	397	rVB	3853732	4129393	64.90%	8.148%
5	6.519	412	414	417	rBV	941311	844429	13.27%	1.666%
6	6.679	425	428	430	rBV	3188883	3466980	54.49%	6.841%
7	7.102	462	465	467	rBV	2782298	3281411	51.57%	6.475%
8	7.810	524	527	529	rBV	1269258	1203748	18.92%	2.375%
9	8.896	618	622	624	rBV	4890867	6363053	100.00%	12.556%
10	9.296	654	657	659	rBV	640522	657950	10.34%	1.298%
11	9.559	677	680	682	rBV	1569753	1744915	27.42%	3.443%
12	10.005	718	719	721	rVB	84671	76402	1.20%	0.151%
13	10.348	746	749	751	rBV	3353225	3535767	55.57%	6.977%
14	10.473	758	760	764	rVB	104552	157912	2.48%	0.312%
15	10.919	797	799	805	rVB2	98641	158986	2.50%	0.314%
16	11.033	806	809	810	rVV	1685593	1655645	26.02%	3.267%
17	11.056	810	811	813	rVB	303808	240184	3.77%	0.474%
18	11.353	834	837	839	rVB2	66453	110615	1.74%	0.218%
19	11.536	848	853	854	rBV3	94971	109268	1.72%	0.216%
20	11.559	854	855	856	rVV	89056	95520	1.50%	0.188%
21	11.594	856	858	861	rVV2	153567	242217	3.81%	0.478%
22	11.639	861	862	868	rVB	117260	192133	3.02%	0.379%
23	12.085	898	901	902	rBV	82611	85471	1.34%	0.169%
24	12.119	902	904	907	rVV2	50363	115761	1.82%	0.228%
25	12.176	907	909	912	rVV	46280	63655	1.00%	0.126%
26	12.234	912	914	917	rVV	405617	501652	7.88%	0.990%
27	12.371	925	926	931	rBV3	32931	69680	1.10%	0.137%
28	12.462	931	934	937	rVV	513249	543965	8.55%	1.073%
29	12.622	945	948	950	rVV	4260687	4817918	75.72%	9.507%
30	12.691	951	954	957	rBV	50373	78428	1.23%	0.155%
31	12.794	960	963	965	rVB	65602	125061	1.97%	0.247%
32	12.897	970	972	976	rVB	77926	102062	1.60%	0.201%
33	13.171	993	996	998	rBV	133494	153309	2.41%	0.303%
34	13.411	1015	1017	1020	rBV3	51260	113709	1.79%	0.224%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.548	1025	1029	1036	rBV3	84063	329145	5.17%	0.649%
36	13.662	1036	1039	1040	rBV2	1258208	1524297	23.96%	3.008%
37	14.051	1068	1073	1075	rBV	67243	111854	1.76%	0.221%
38	14.302	1094	1095	1097	rBV	56876	79927	1.26%	0.158%
39	14.394	1097	1103	1104	rVV3	35984	102047	1.60%	0.201%
40	14.451	1104	1108	1111	rVB5	38301	113277	1.78%	0.224%
41	14.508	1111	1113	1116	rBV3	46390	89541	1.41%	0.177%
42	14.657	1123	1126	1131	rVV	199383	356191	5.60%	0.703%
43	14.737	1131	1133	1136	rVB2	94703	133251	2.09%	0.263%
44	14.908	1146	1148	1151	rVB	129354	134465	2.11%	0.265%
45	14.965	1151	1153	1155	rVV	125510	185152	2.91%	0.365%
46	15.011	1155	1157	1163	rVB	798765	1089469	17.12%	2.150%
47	15.400	1188	1191	1194	rBV2	61253	109092	1.71%	0.215%
48	16.223	1261	1263	1273	rVB2	71295	210950	3.32%	0.416%
49	16.588	1292	1295	1304	rVB	59956	132185	2.08%	0.261%
50	16.805	1311	1314	1320	rVB3	27947	71832	1.13%	0.142%

Sum of corrected areas: 50678589

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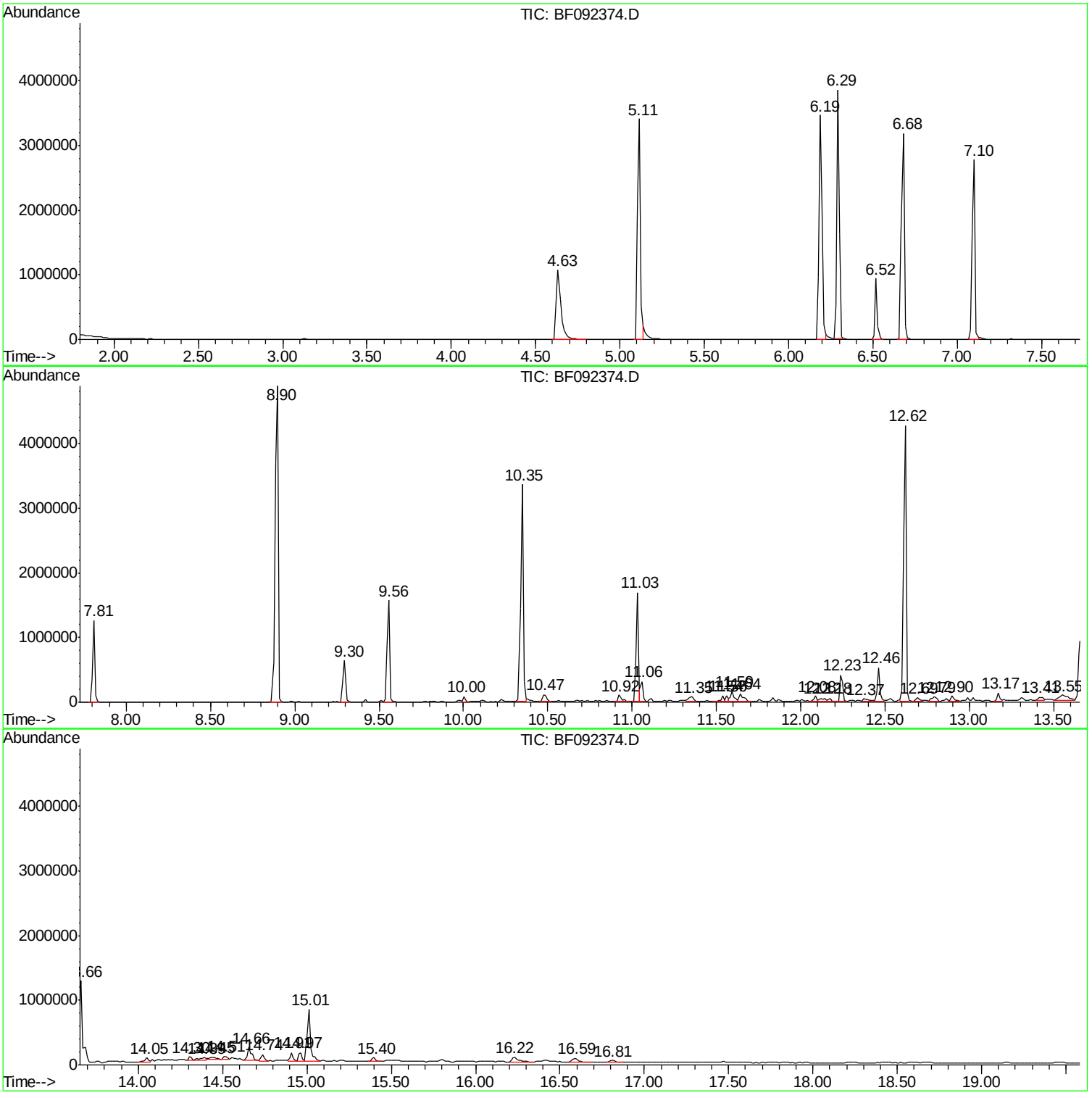
Instrument :
BNA_F
ClientSampleId :
ROLL-OFF-15939-COMP

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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

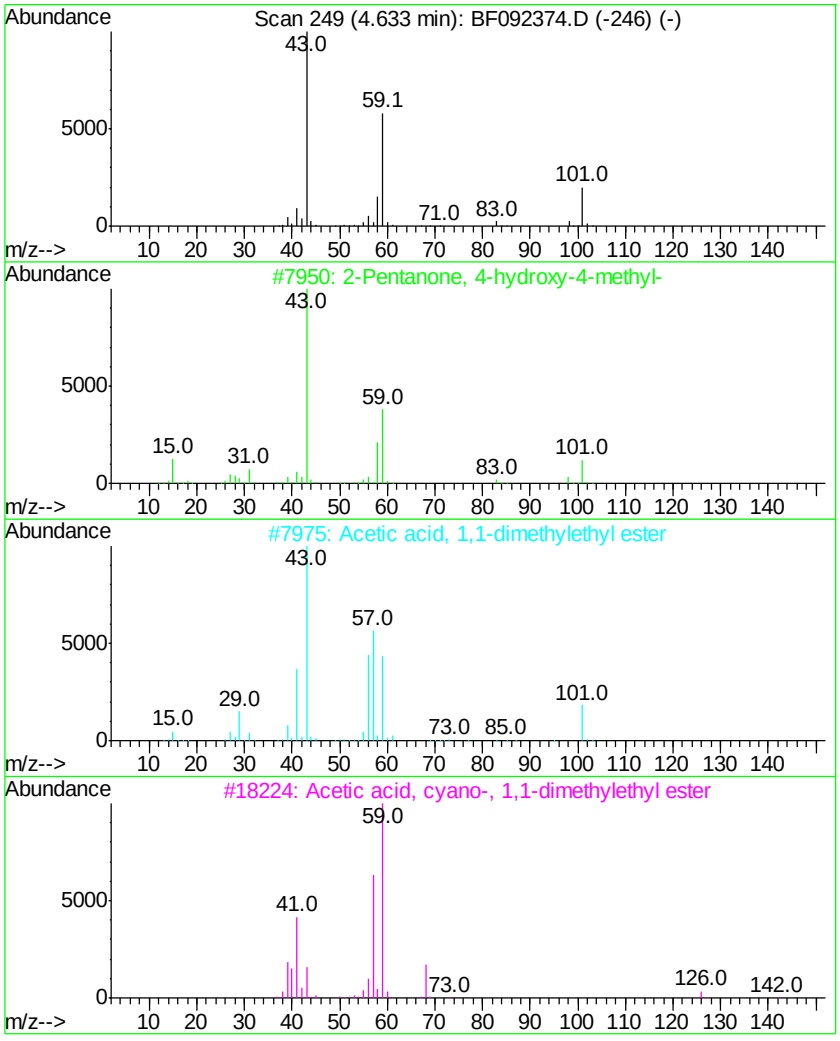
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

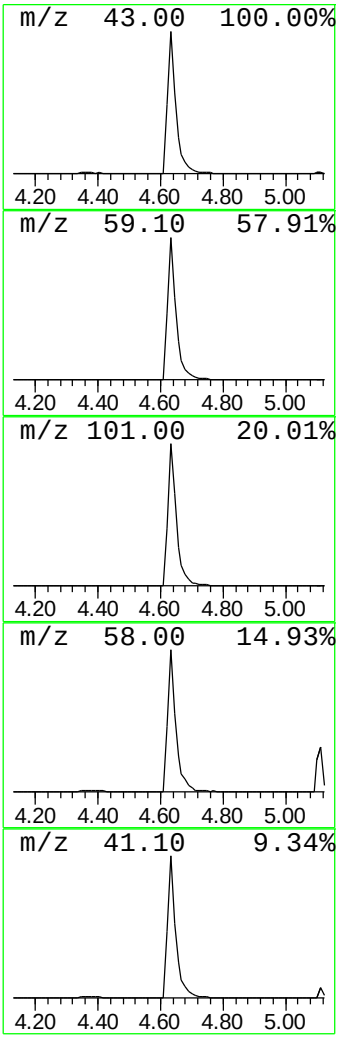
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	46.00 ng	1941980	1,4-Dichlorobenzene-d4	6.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
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Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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

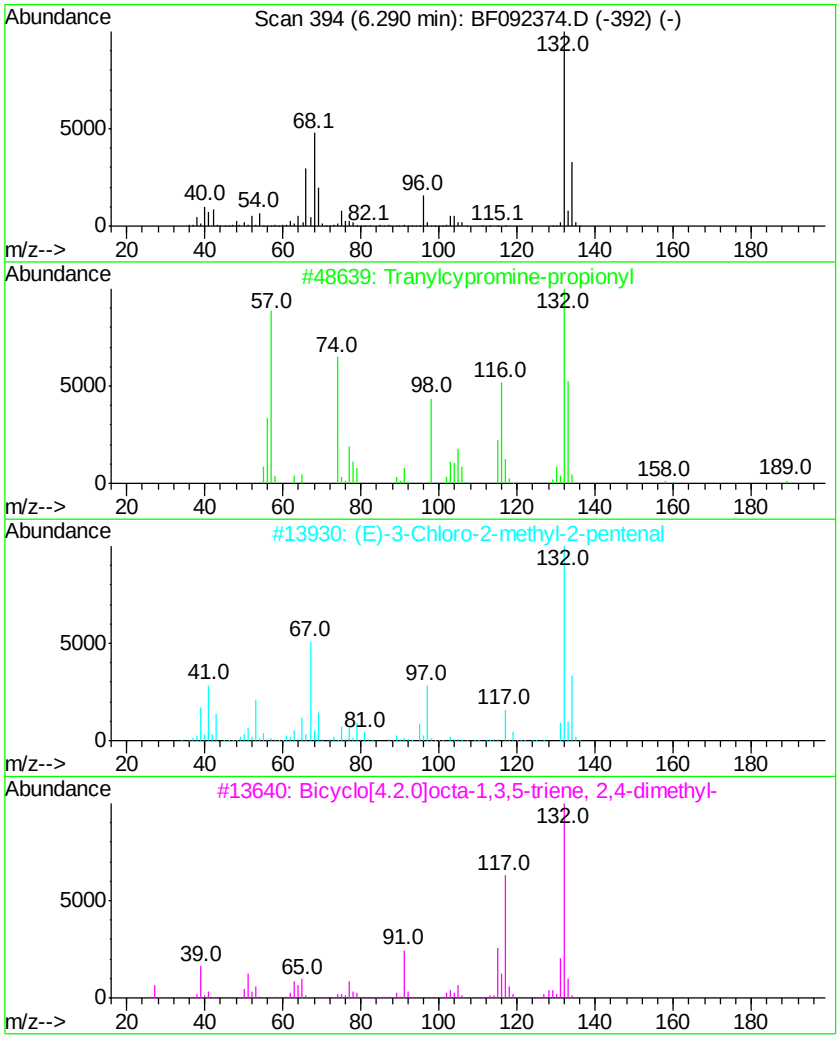
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

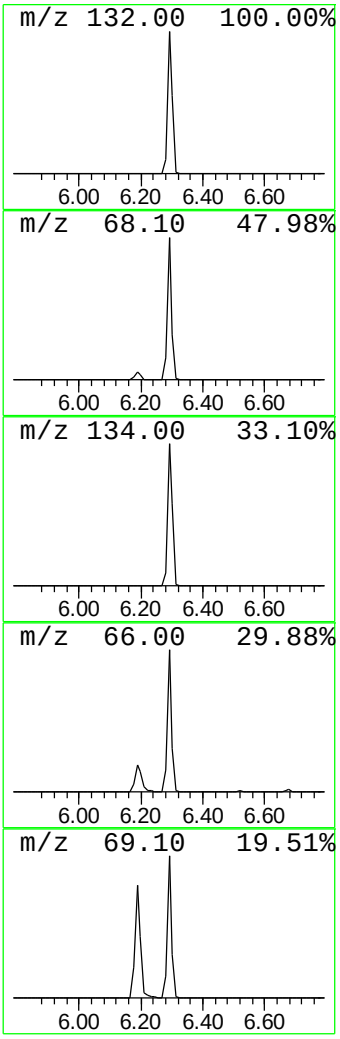
****

Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	97.80 ng	4129390	1,4-Dichlorobenzene-d4	6.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
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	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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

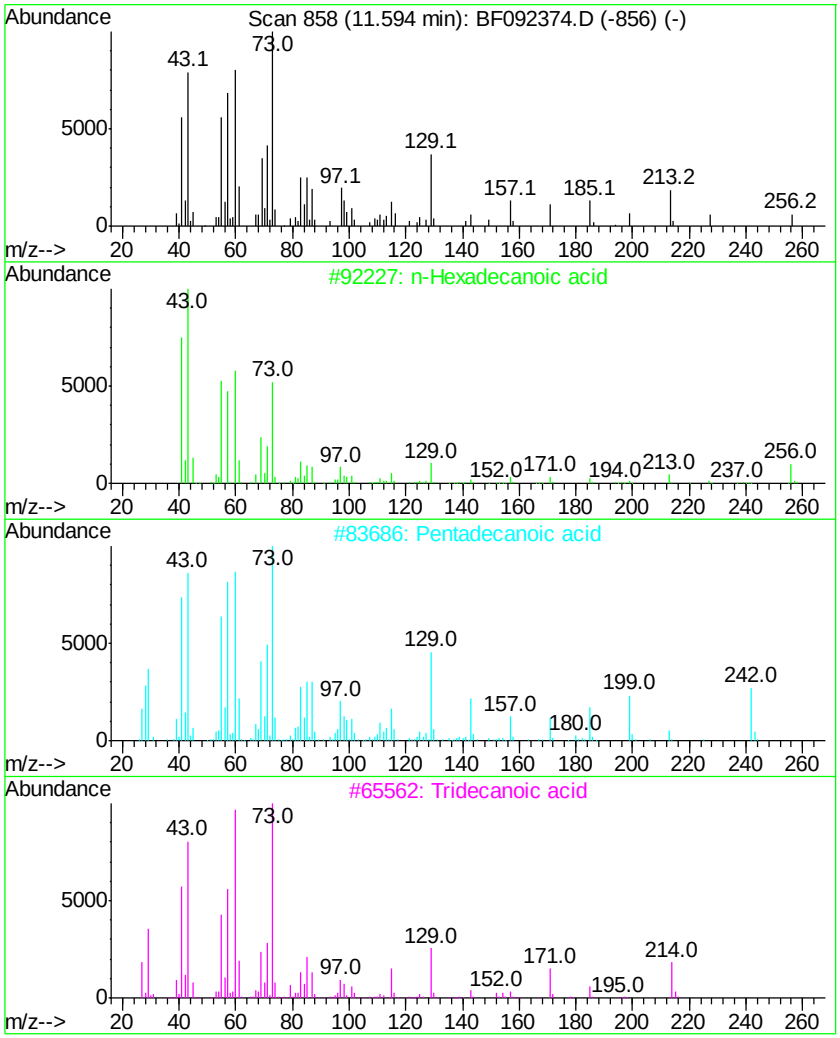
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

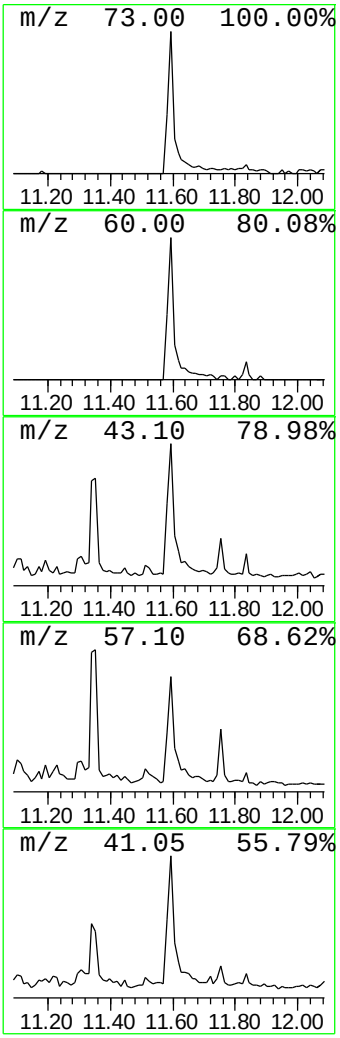
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.93 ng	242217	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecane	170	C12H26	000112-40-3	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
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Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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

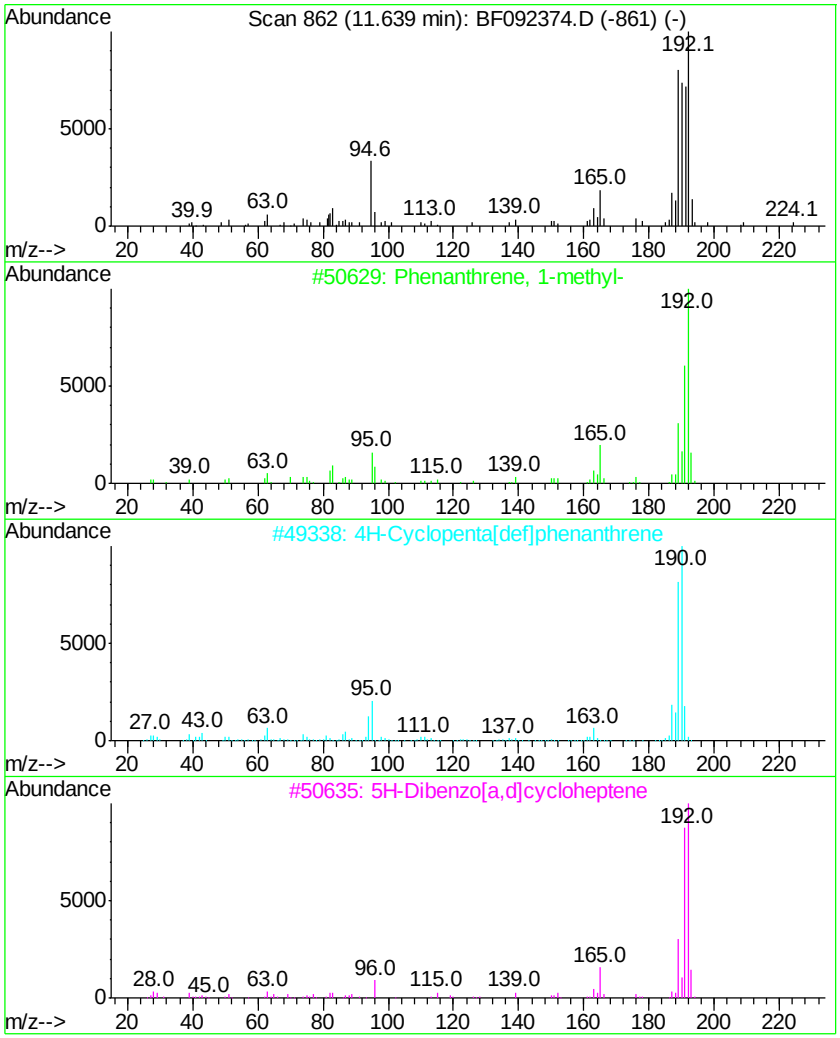
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

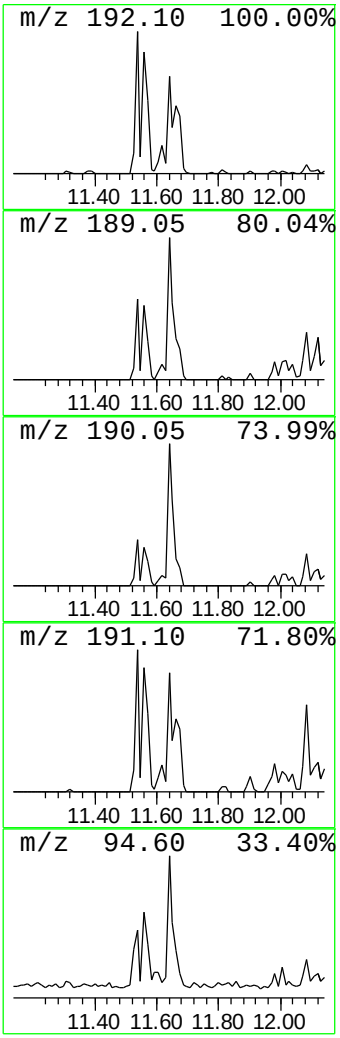
****

Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.64	2.32 ng	192133	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	55
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	46
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	45
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42





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Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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

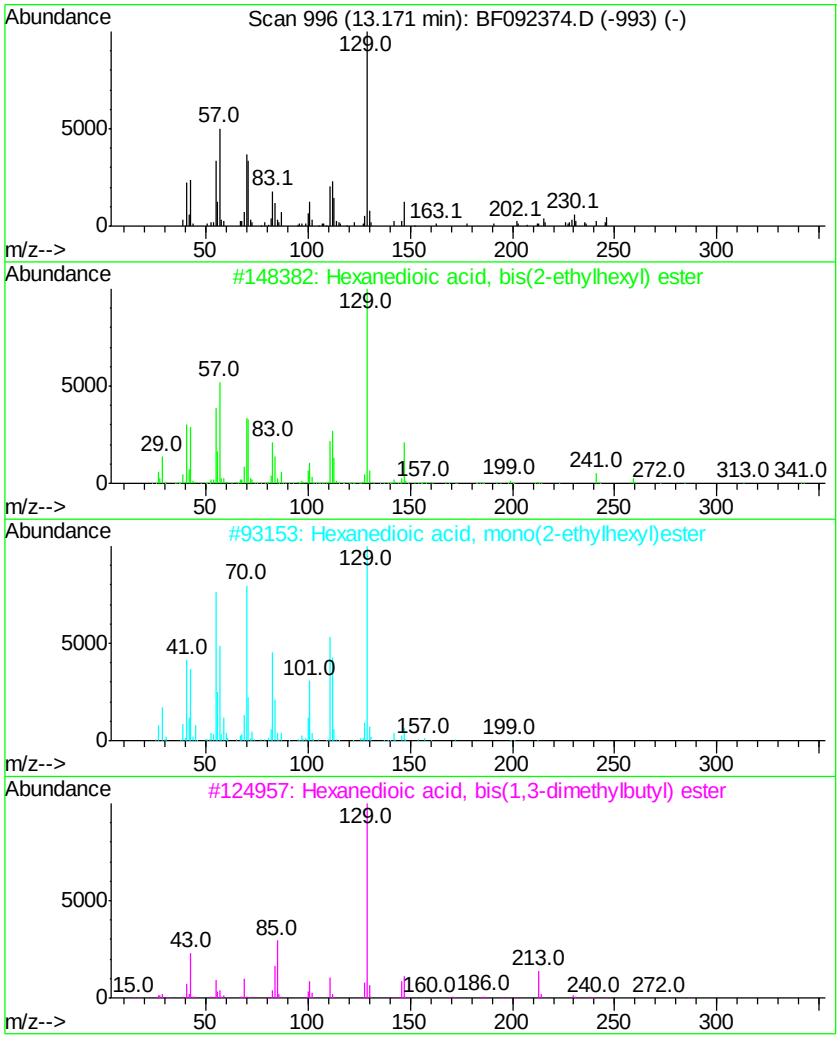
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

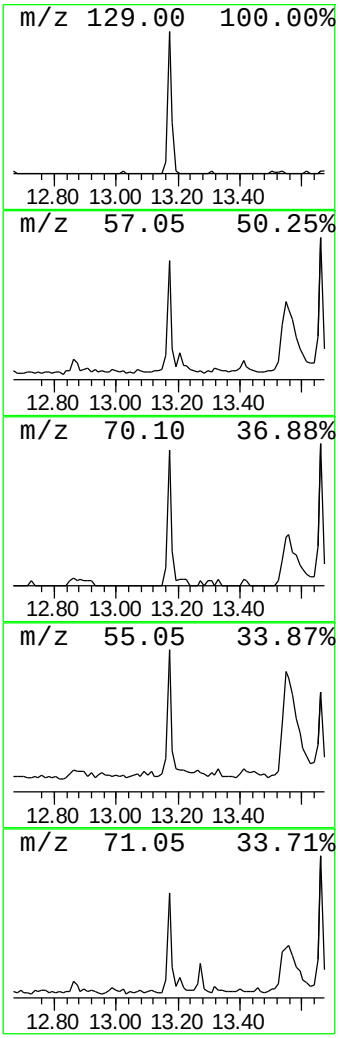
****

Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	2.01 ng	153309	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	46
3	Hexanedioic acid, bis(1,3-dimeth...	314	C18H34O4	055125-22-9	40
4	Hexanedioic acid, dihexyl ester	314	C18H34O4	000110-33-8	38
5	2,6-Difluoroaniline	129	C6H5F2N	005509-65-9	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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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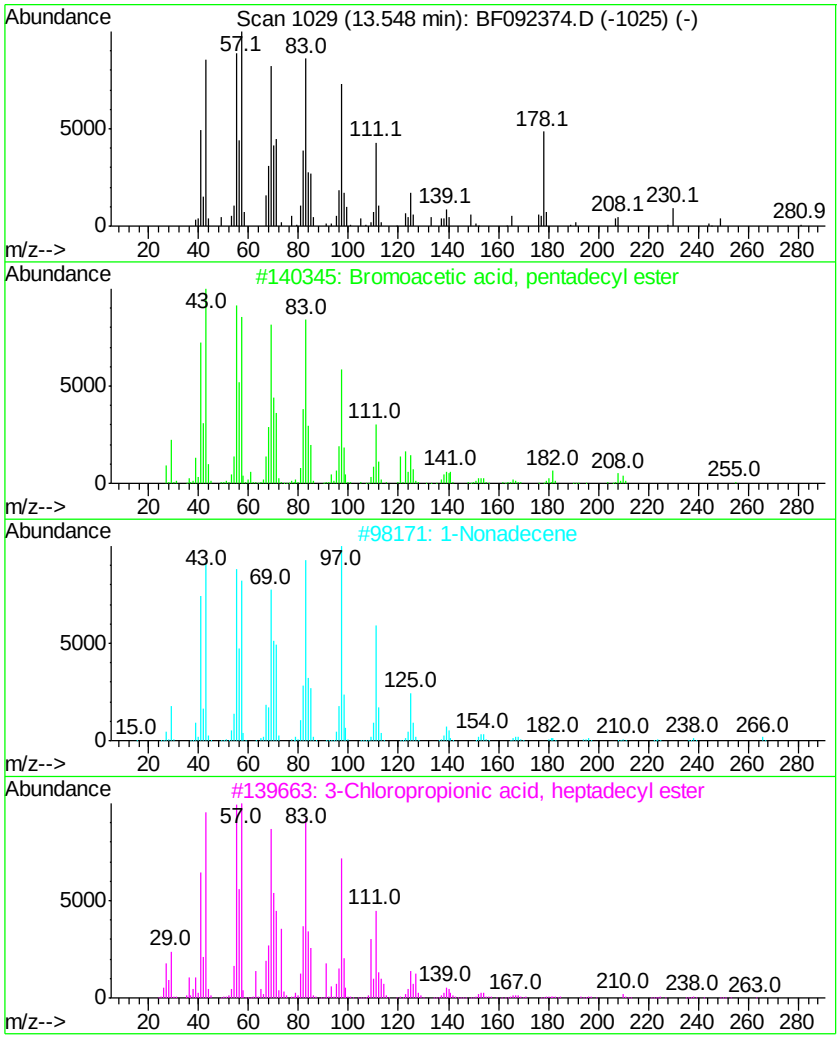
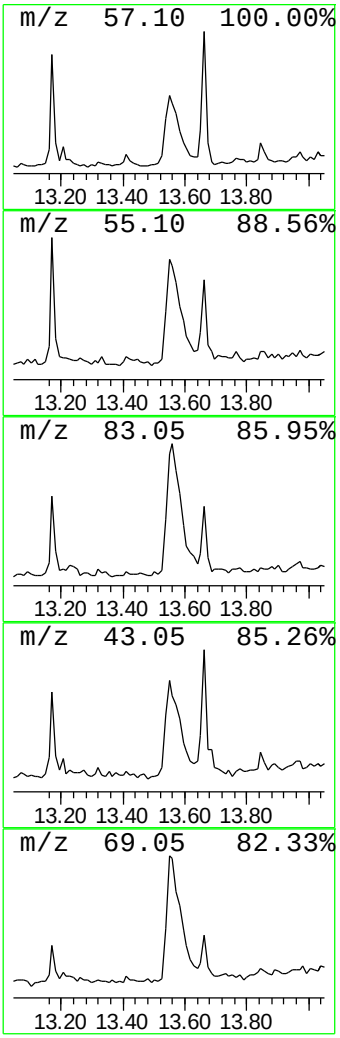
Peak Number 7 Bromoacetic acid, pentadecy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	4.32 ng	329145	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
2	1-Nonadecene	266	C19H38	018435-45-5	87
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	87
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87





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Misc :
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Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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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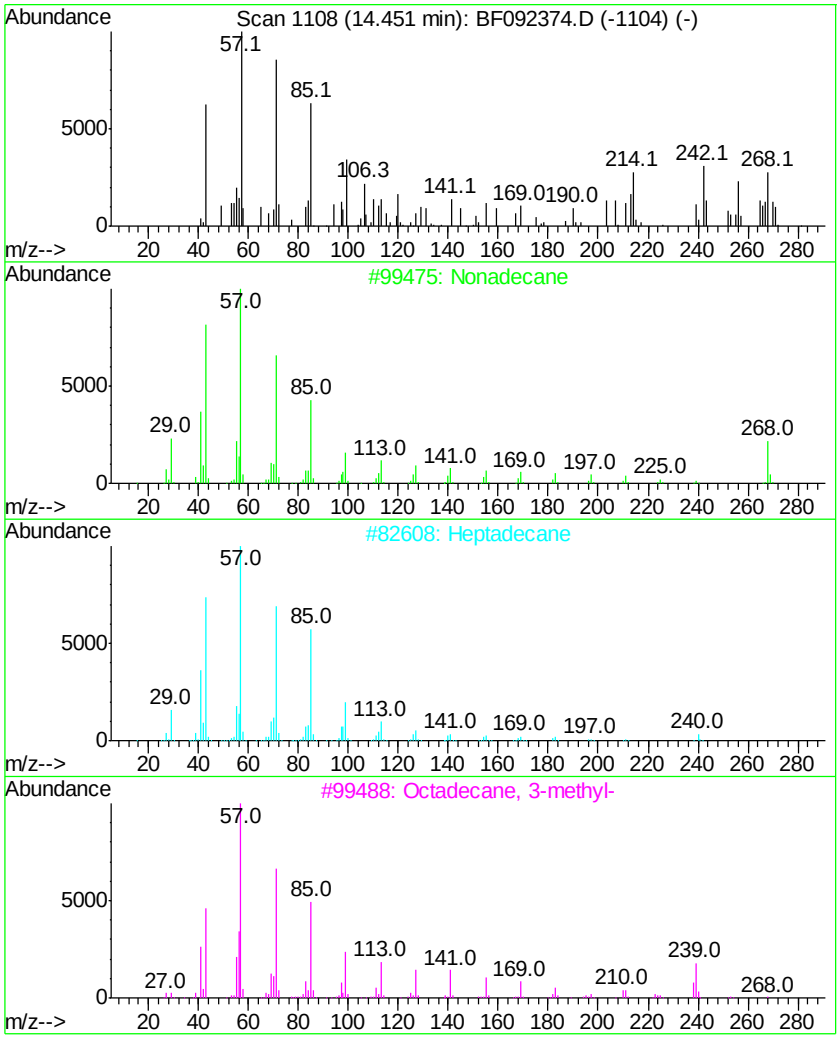
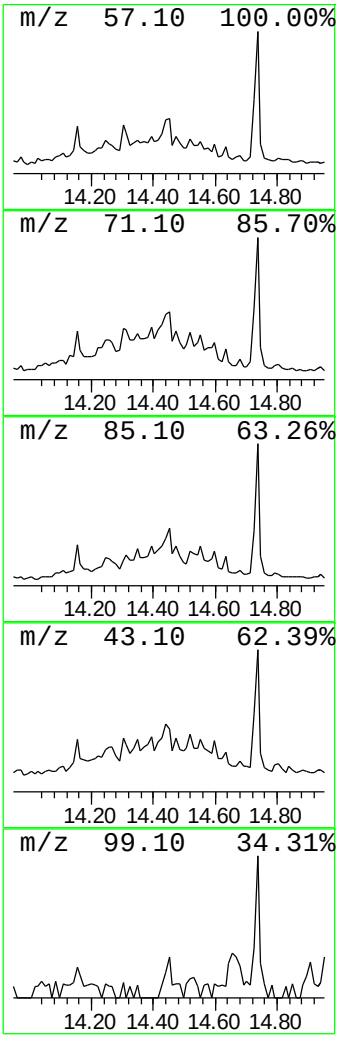
Peak Number 8 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.08 ng	113277	Perylene-d12	15.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	60
2	Heptadecane	240	C17H36	000629-78-7	50
3	Octadecane, 3-methyl-	268	C19H40	006561-44-0	38
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	38
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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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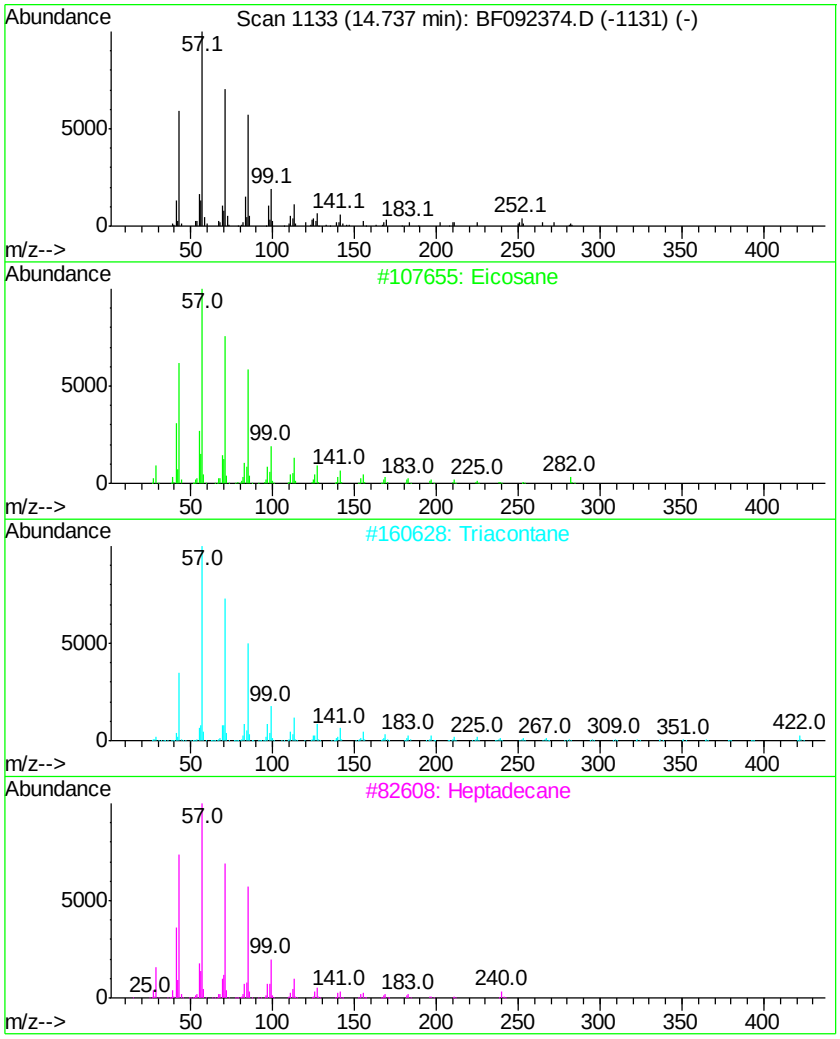
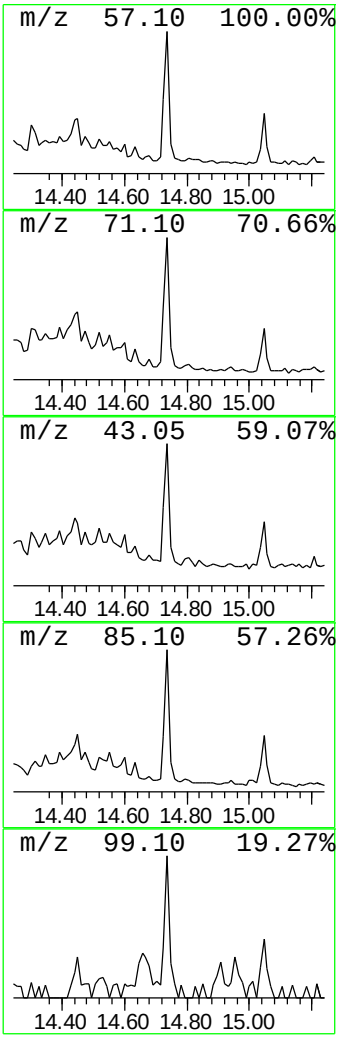
Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	2.45 ng	133251	Perylene-d12	15.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Triacontane	422	C30H62	000638-68-6	86
3	Heptadecane	240	C17H36	000629-78-7	86
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5	Nonacosane	408	C29H60	000630-03-5	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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

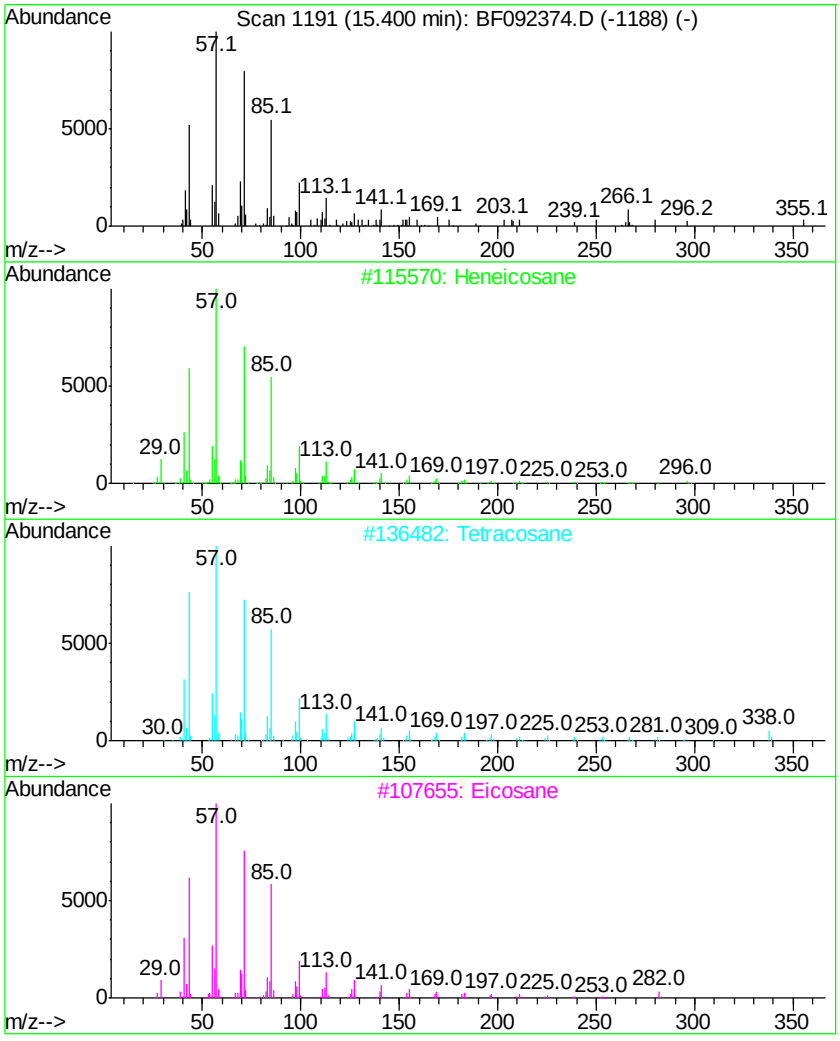
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

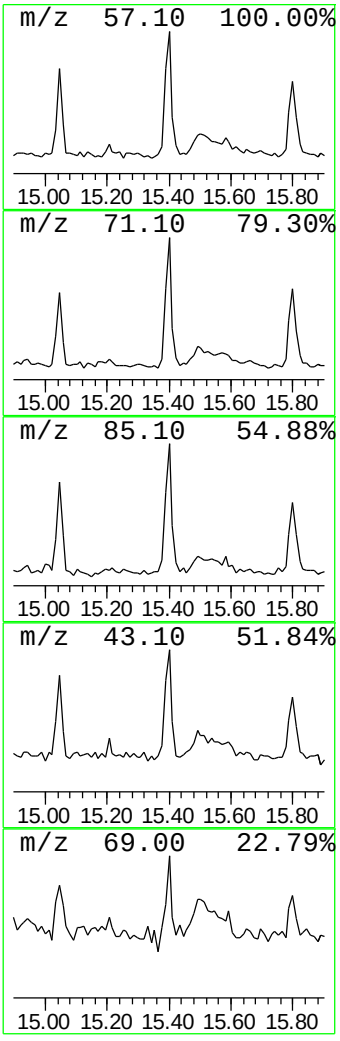
****

Peak Number 11 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	2.00 ng	109092	Perylene-d12	15.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Tetracosane	338	C24H50	000646-31-1	86
3	Eicosane	282	C20H42	000112-95-8	86
4	Docosane	310	C22H46	000629-97-0	86
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092374.D
Acq On : 20 Jan 2017 15:50
Operator : UM/SJ
Sample : I1304-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ROLL-OFF-15939-COMP

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...	4.63	46.0	ng	1941980	1	6.52	844429	20.0
unknown6.29	6.29	97.8	ng	4129390	1	6.52	844429	20.0
n-Hexadecanoic acid	11.59	2.9	ng	242217	4	11.03	1655650	20.0
Phenanthrene, 1-m...	11.64	2.3	ng	192133	4	11.03	1655650	20.0
Hexanedioic acid,...	13.17	2.0	ng	153309	5	13.66	1524300	20.0
Bromoacetic acid,...	13.55	4.3	ng	329145	5	13.66	1524300	20.0
Nonadecane	14.45	2.1	ng	113277	6	15.01	1089470	20.0
Eicosane	14.74	2.5	ng	133251	6	15.01	1089470	20.0
Heneicosane	15.40	2.0	ng	109092	6	15.01	1089470	20.0