LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-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-BF031816.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	5.041	239	241	250	rBV	225334	383441	9.86%	1.014%
2	5.453	274	277	280	rBV	2710045	3445845	88.58%	9.115%
3	6.493	364	368	370	rBV	3001269	3890019	100.00%	10.290%
4	6.619	376	379	382	rBV	3011681	3590447	92.30%	9.498%
5	6.847	397	399	402	rBV	729543	801346	20.60%	2.120%
6	7.007	410	413	416	rBV	2853272	2820196	72.50%	7.460%
7	7.419	446	449	451	rBV	2314105	2438913	62.70%	6.452%
8	8.139	509	512	514	rBV	1200774	1134043	29.15%	3.000%
9	9.213	603	606	609	rBV	3726688	3878175	99.70%	10.259%
10	9.602	638	640	642	rBV	301992	335214	8.62%	0.887%
11	9.819	657	659	663	rBV	52354	63859	1.64%	0.169%
12	9.888	663	665	667	rVV	1262399	1156106	29.72%	3.058%
13	10.322	701	703	705	rVB	132575	105023	2.70%	0.278%
14	10.539	719	722	725	rBV	43897	74695	1.92%	0.198%
15	10.676	731	734	737	rBV2	1893962	2532092	65.09%	6.698%
16	10.791	743	744	751	rBV	114804	177269	4.56%	0.469%
17	11.248	781	784	785	rBV	42961	59447	1.53%	0.157%
18	11.374	793	795	796	rBV	1419442	1214207	31.21%	3.212%
19	11.396	796	797	799	rVV	199263	153619	3.95%	0.406%
20	11.899	840	841	844	rBV2	133445	188330	4.84%	0.498%
21	11.979	847	848	853	rVB2	36902	71677	1.84%	0.190%
22	12.585	898	901	903	rBV	287522	301703	7.76%	0.798%
23	12.688	908	910	913	rBV2	60764	101478	2.61%	0.268%
24	12.779	916	918	919	rBV	323803	295164	7.59%	0.781%
25	12.814	919	921	922	rVB	246351	268322	6.90%	0.710%
26	12.962	931	934	936	rVB	3671809	3561193	91.55%	9.420%
27	13.031	936	940	944	rVB3	22238	44249	1.14%	0.117%
28	13.134	946	949	951	rVB	30693	60669	1.56%	0.160%
29	13.191	951	954	957	rBV2	90664	120767	3.10%	0.319%
30	13.237	957	958	962	rVB2	27932	42243	1.09%	0.112%
31	13.488	978	980	981	rBV	168664	170395	4.38%	0.451%
32	13.534	981	984	985	rBV	133036	133580	3.43%	0.353%
33	13.751	1000	1003	1005	rBV4	29584	55227	1.42%	0.146%
34	13.854	1010	1012	1021	rVV	450916	860204	22.11%	2.276%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-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-BF031816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.002	1022	1025	1032	rVB2	814166	1176051	30.23%	3.111%
36	14.174	1038	1040	1043	rVB	189258	164307	4.22%	0.435%
37	14.482	1064	1067	1068	rBV	112321	134175	3.45%	0.355%
38	14.517	1068	1070	1074	rVB3	32259	62080	1.60%	0.164%
39	14.780	1090	1093	1096	rBV	69375	88280	2.27%	0.234%
40	15.020	1112	1114	1119	rBV	126420	271351	6.98%	0.718%
41	15.100	1119	1121	1122	rBV	41431	42308	1.09%	0.112%
42	15.317	1137	1140	1143	rVB	71675	100917	2.59%	0.267%
43	15.374	1143	1145	1148	rVV	112077	143522	3.69%	0.380%
44	15.431	1148	1150	1157	rVB	576712	796641	20.48%	2.107%
45	15.968	1192	1197	1201	rBV5	20317	78067	2.01%	0.207%
46	16.825	1269	1272	1276	rVB2	44308	86319	2.22%	0.228%
47	17.054	1289	1292	1298	rBV5	14565	41709	1.07%	0.110%
48	17.237	1305	1308	1313	rVB	37716	87872	2.26%	0.232%

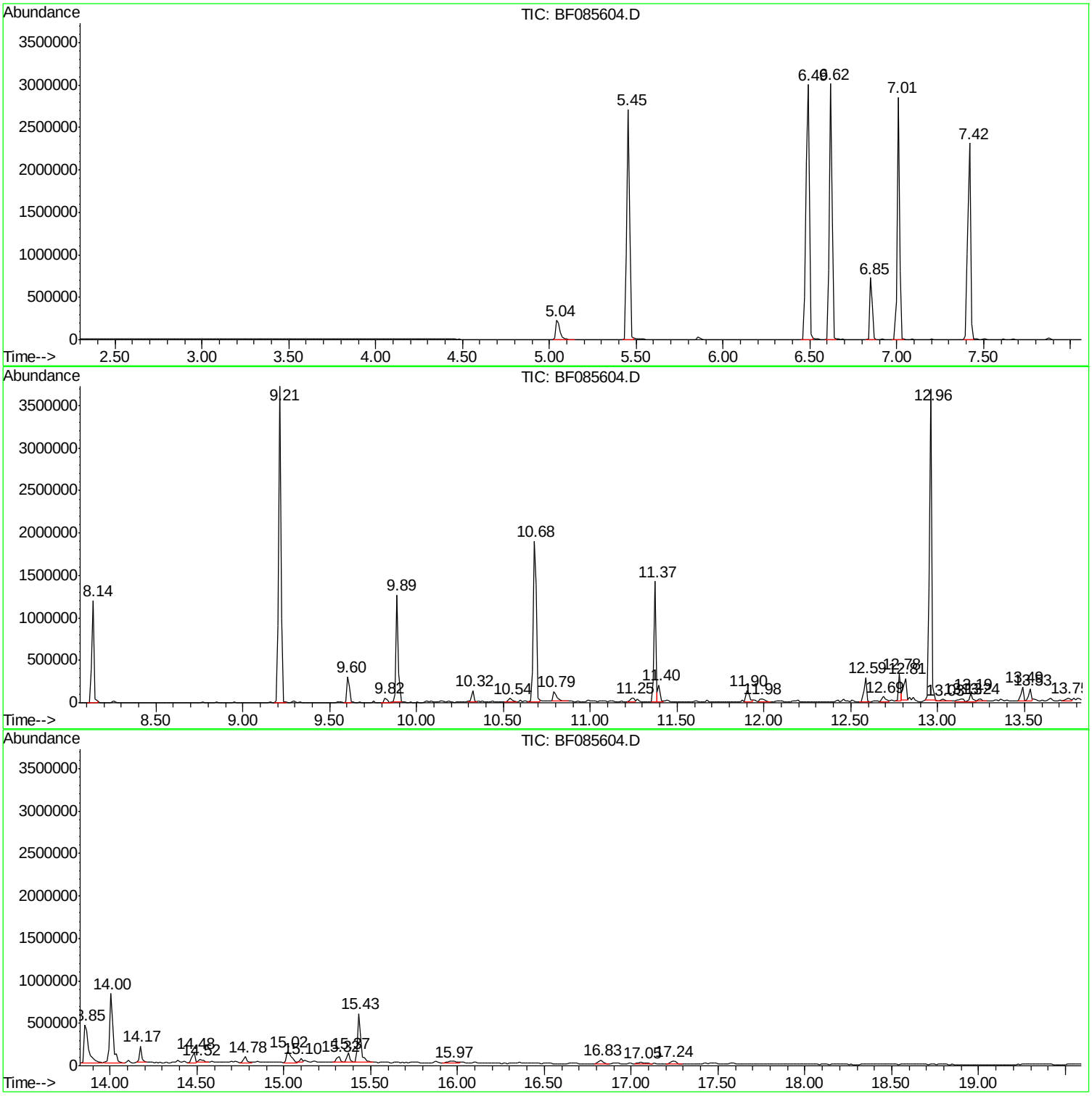
Sum of corrected areas: 37802756

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.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\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

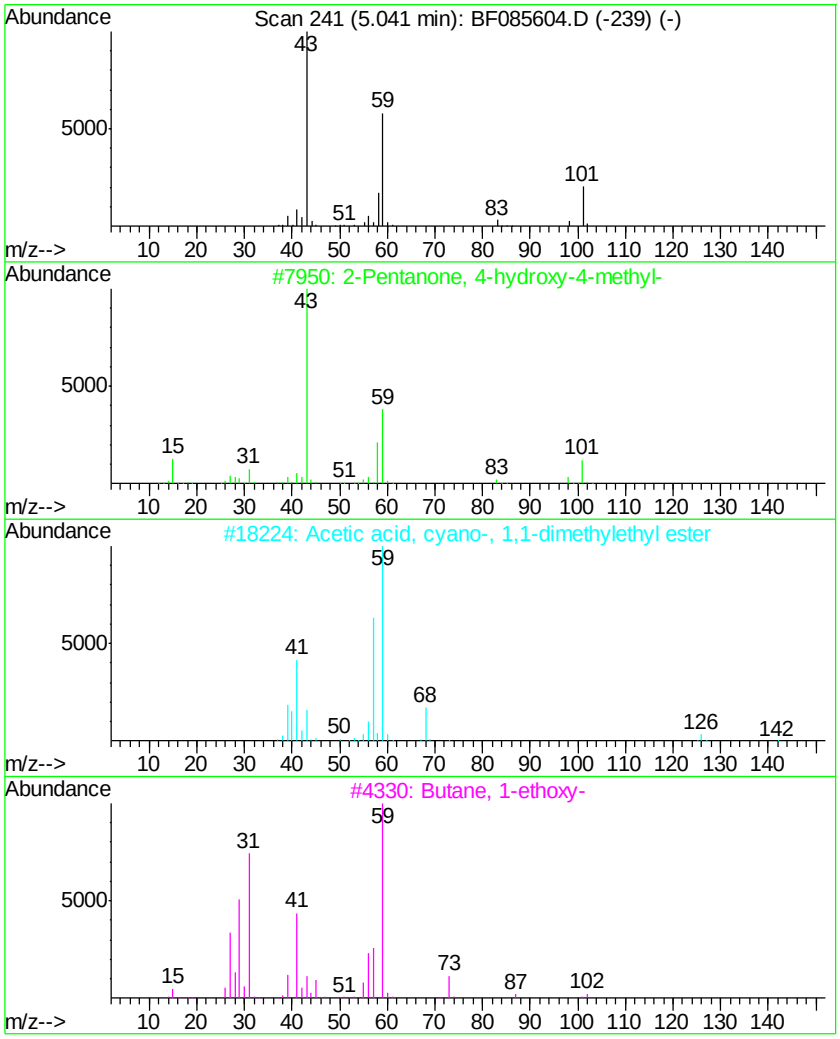
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

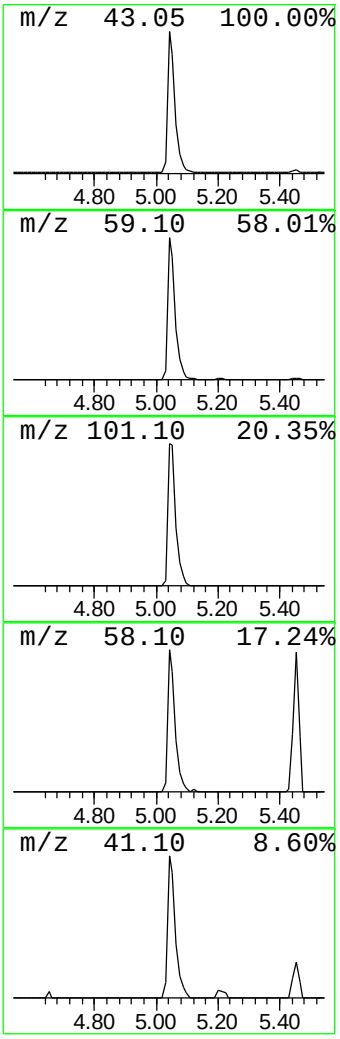
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	9.57 ng	383441	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

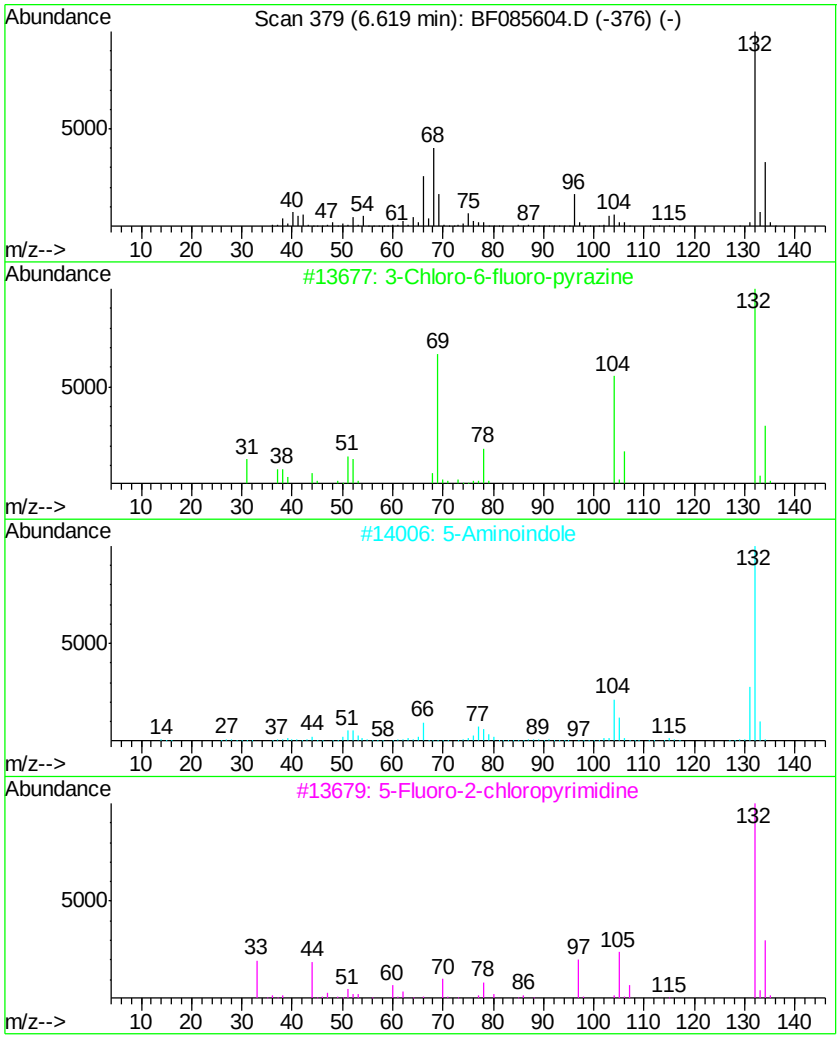
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

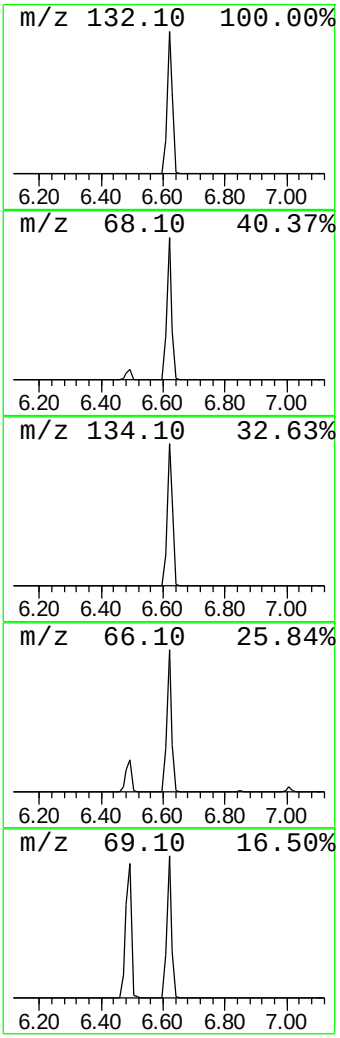
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	89.61 ng	3590450	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

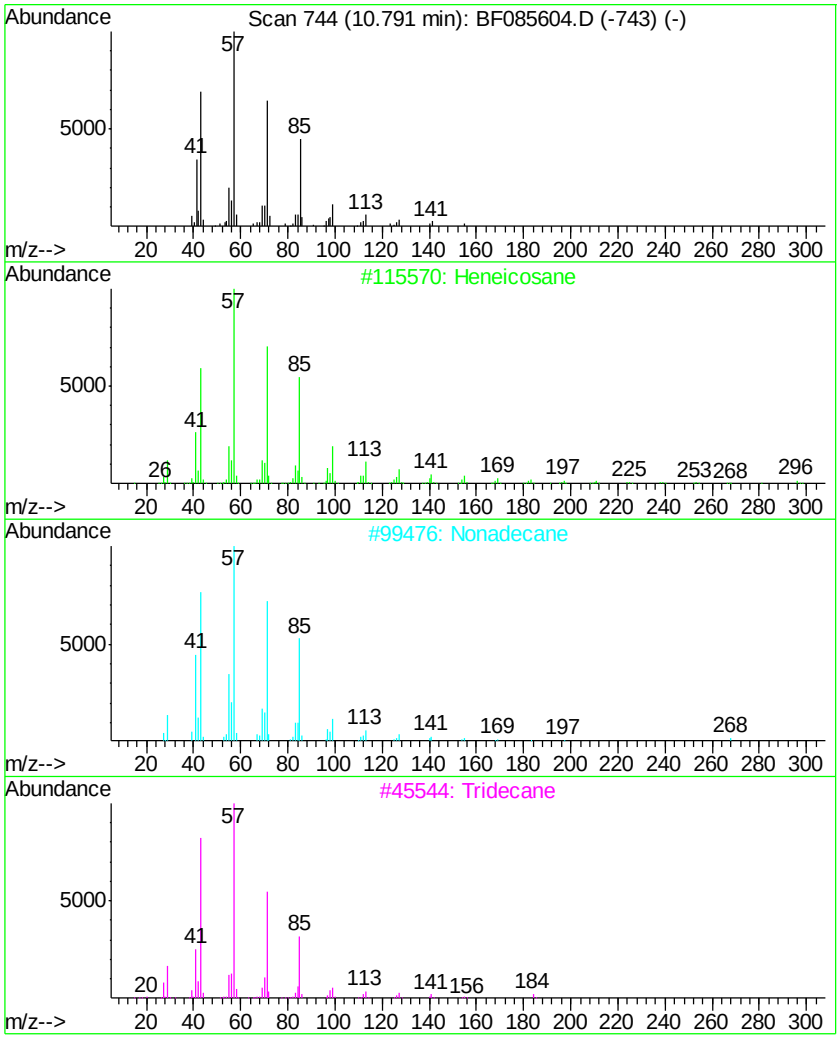
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

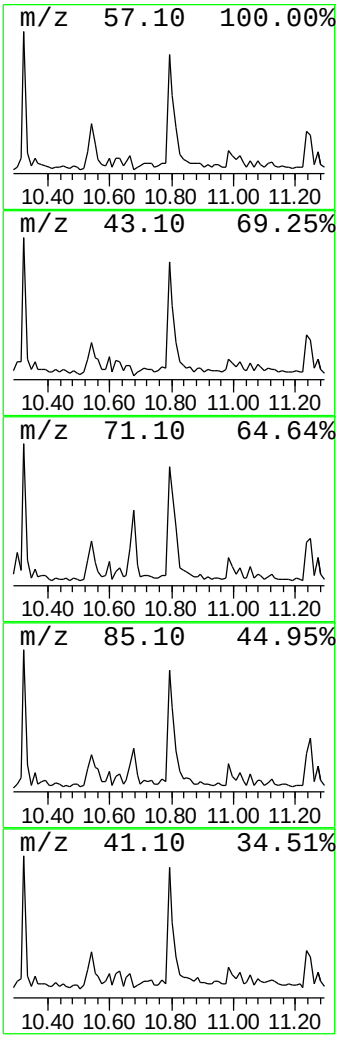
****

Peak Number 4 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	2.92 ng	177269	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Nonadecane	268	C19H40	000629-92-5	87
3	Tridecane	184	C13H28	000629-50-5	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Tetradecane	198	C14H30	000629-59-4	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

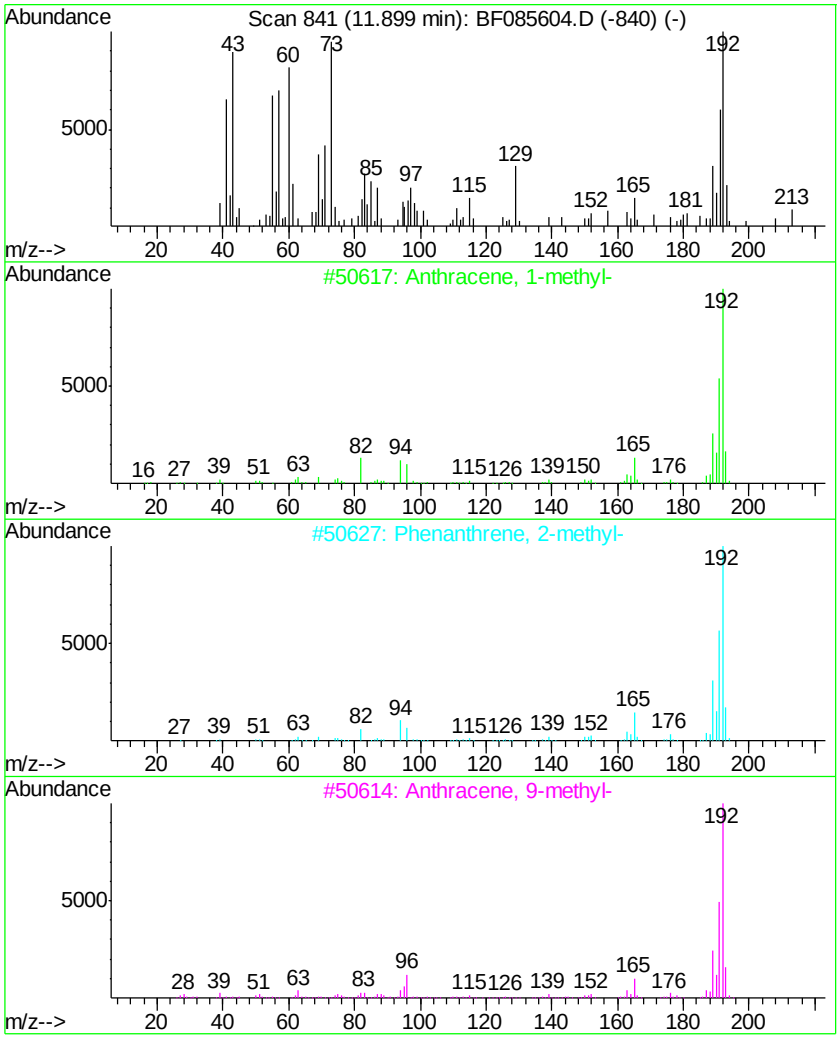
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

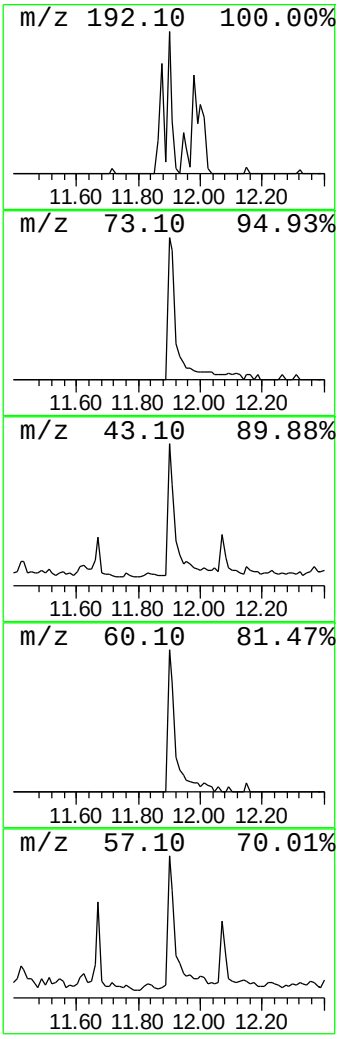
****

Peak Number 5 Anthracene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.10 ng	188330	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	86
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	80
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	72
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	50





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

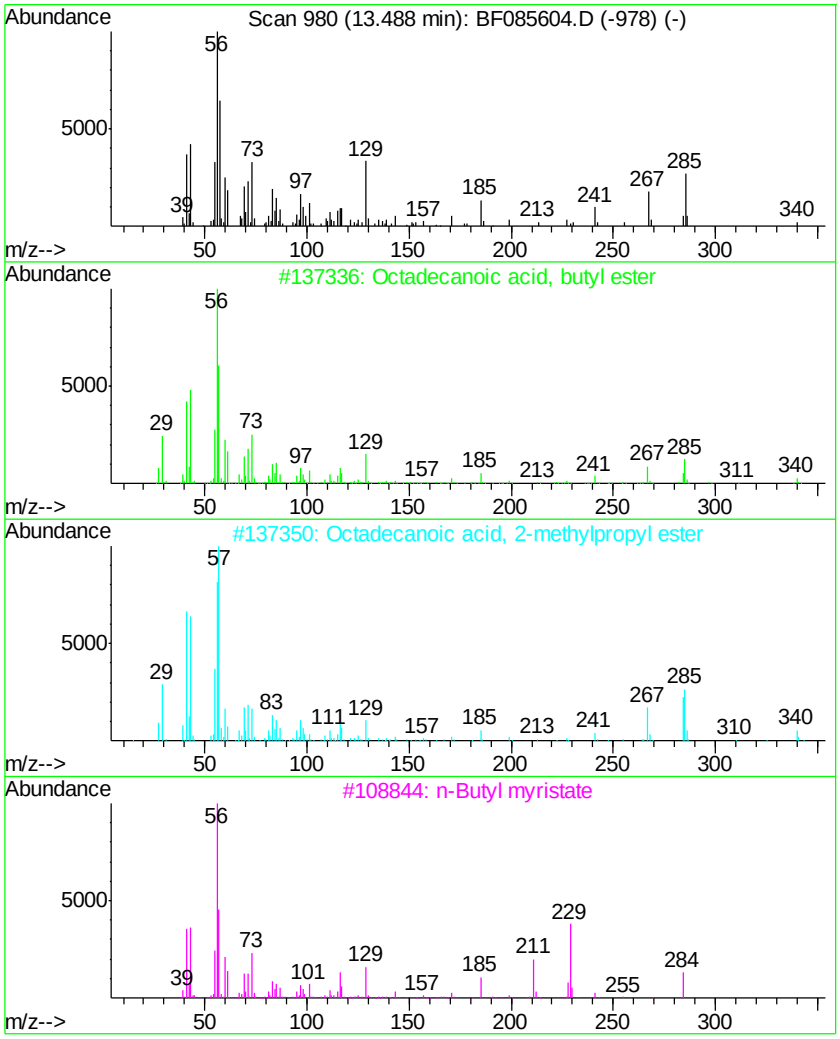
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

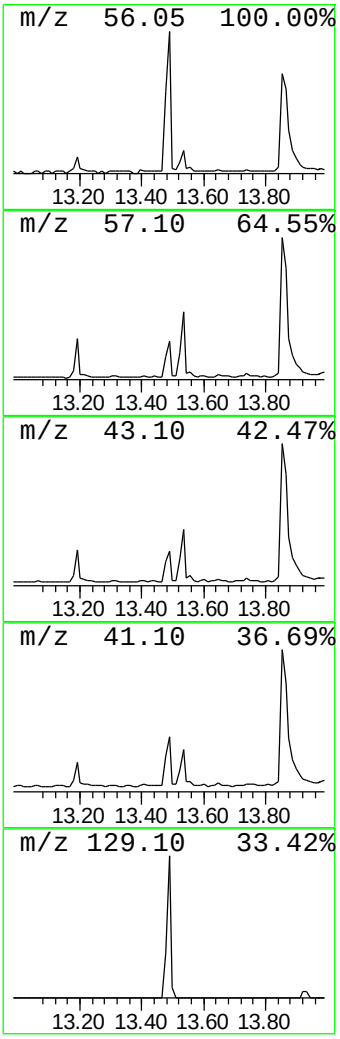
****

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.90 ng	170395	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	80
3	n-Butyl myristate	284	C18H36O2	000110-36-1	52
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	7-Methyl-octadecan-7-ol	284	C19H40O	1000194-50-8	32





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

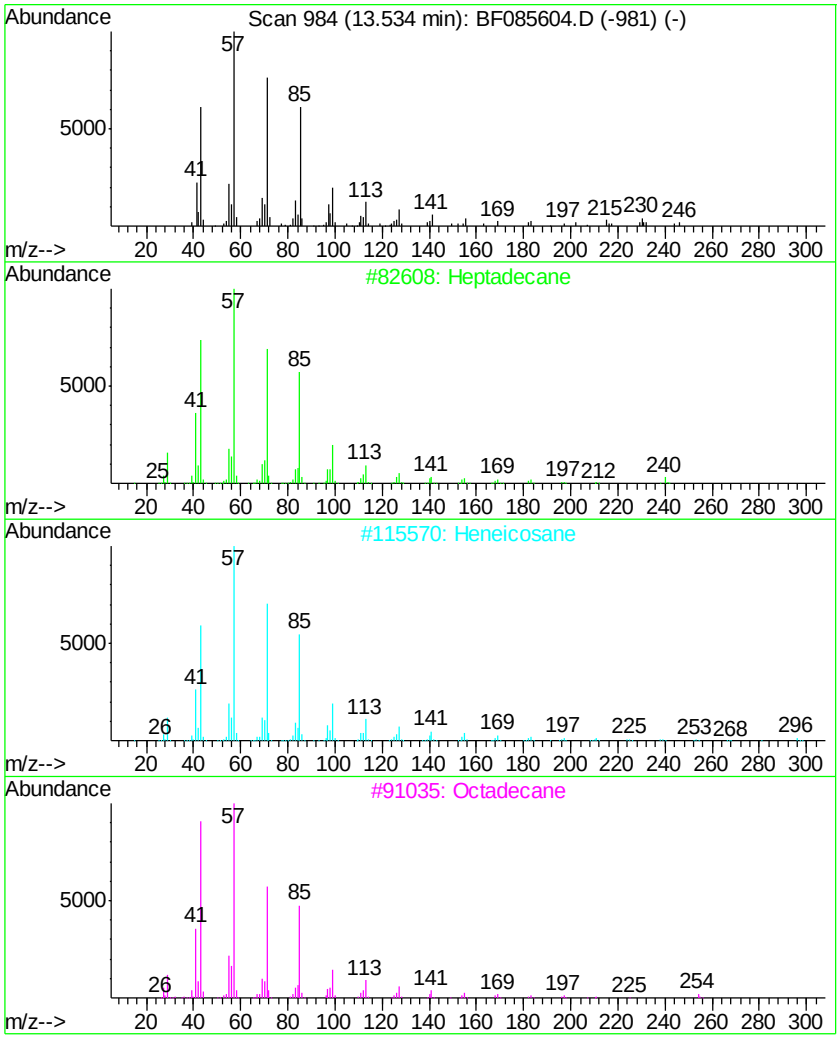
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

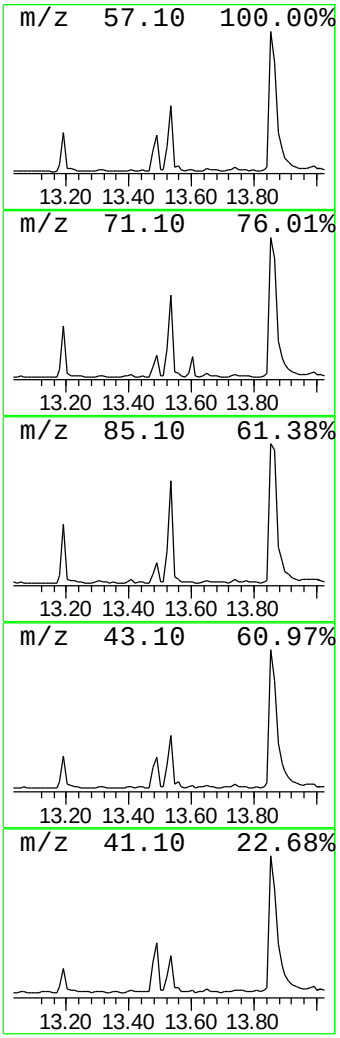
****

Peak Number 8 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	2.27 ng	133580	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Octadecane	254	C18H38	000593-45-3	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Pentacosane	352	C25H52	000629-99-2	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

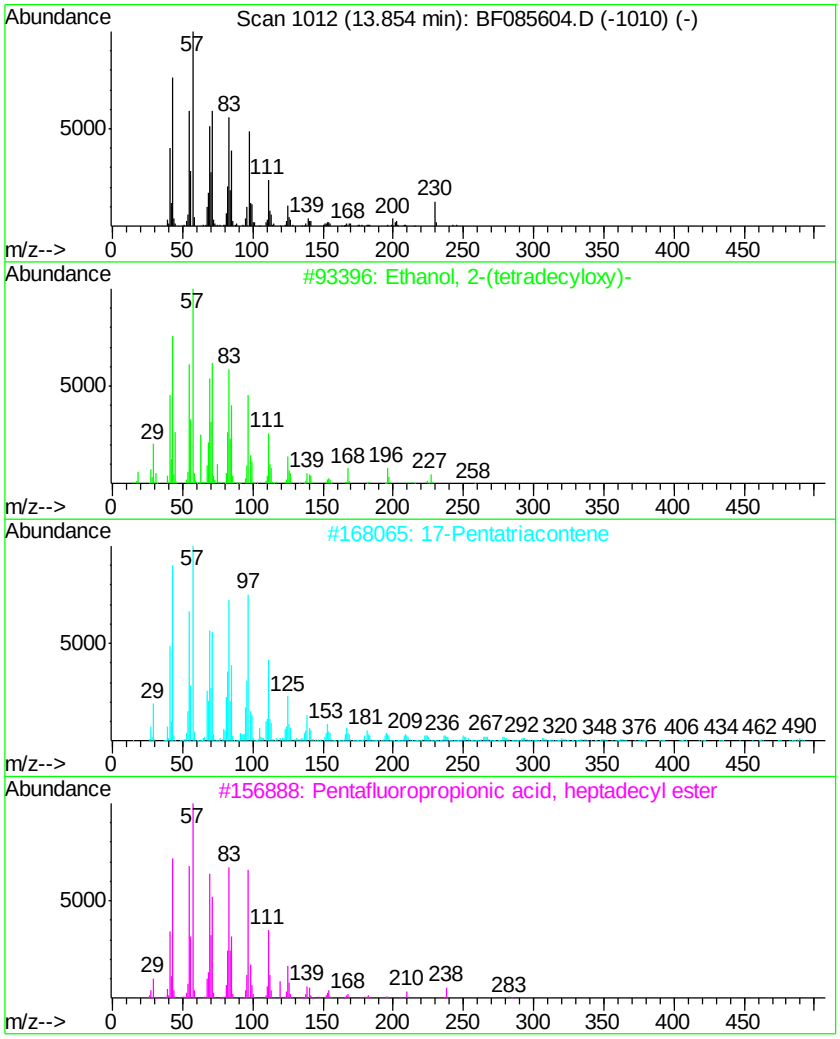
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

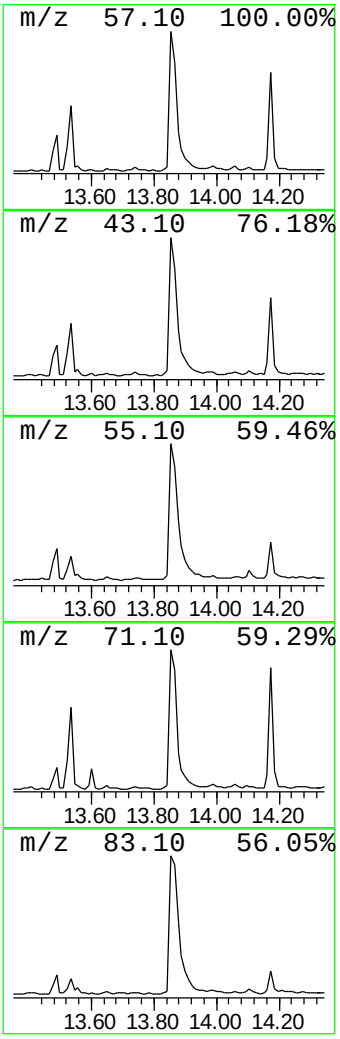
****

Peak Number 9 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	14.63 ng	860204	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	86
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	81
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	70
5	1-Nonadecanol	284	C19H40O	001454-84-8	70





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

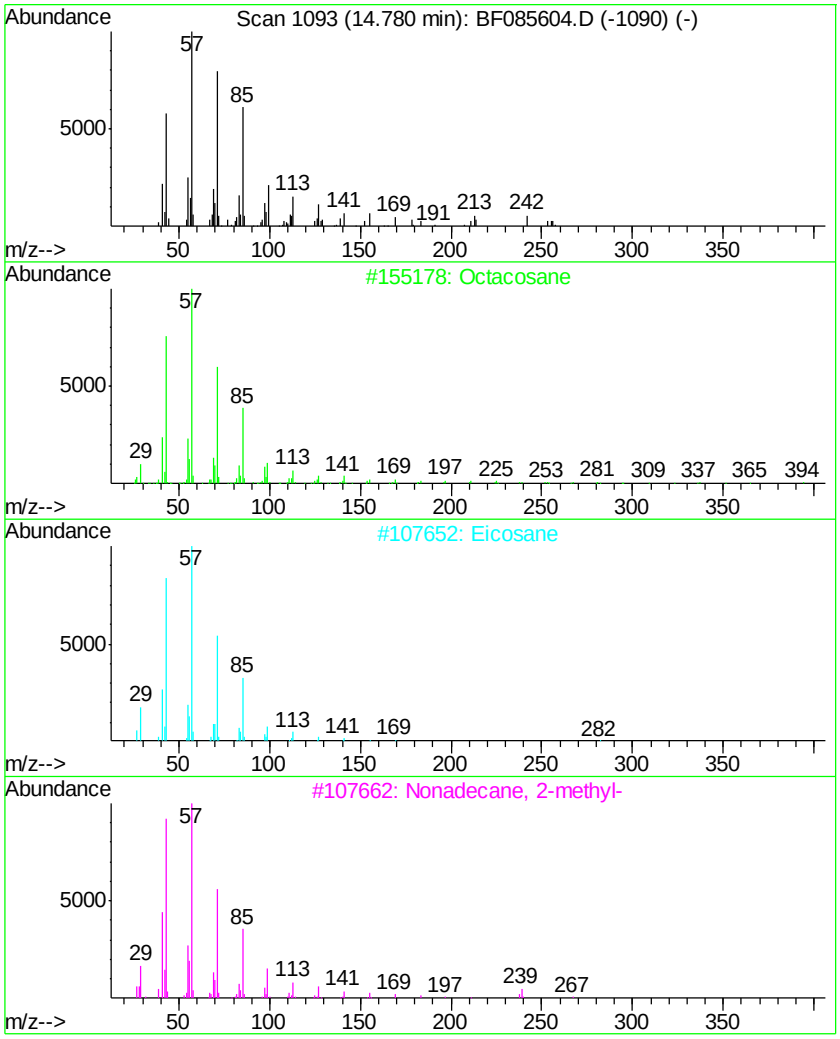
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

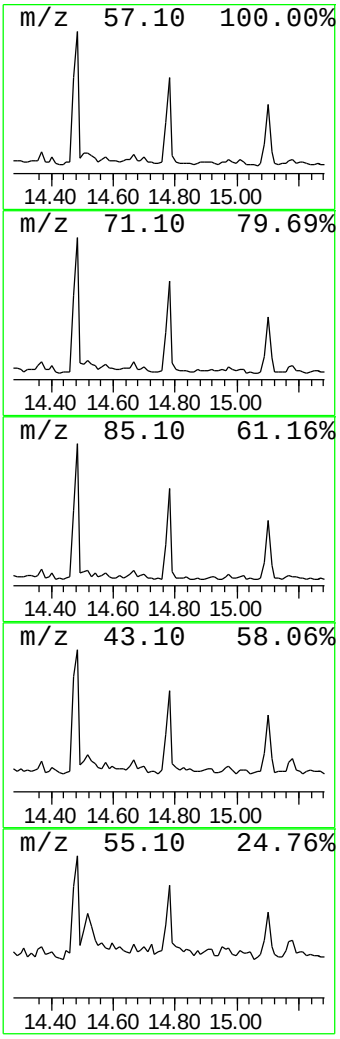
****

Peak Number 12 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	2.22 ng	88280	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Eicosane	282	C20H42	000112-95-8	87
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	87
4	Heptadecane	240	C17H36	000629-78-7	87
5	Hexacosane	366	C26H54	000630-01-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031816\
Data File : BF085604.D
Acq On : 20 Mar 2016 8:02
Operator : UM/SJ
Sample : H1815-16
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.04	9.6	ng	383441	1	6.85	801346	20.0
unknown6.62	6.62	89.6	ng	3590450	1	6.85	801346	20.0
Heneicosane	10.79	2.9	ng	177269	4	11.37	1214210	20.0
Anthracene, 1-met...	11.90	3.1	ng	188330	4	11.37	1214210	20.0
Octadecanoic acid...	13.49	2.9	ng	170395	5	14.00	1176050	20.0
Heptadecane	13.53	2.3	ng	133580	5	14.00	1176050	20.0
Ethanol, 2-(tetra...	13.85	14.6	ng	860204	5	14.00	1176050	20.0
Octacosane	14.78	2.2	ng	88280	6	15.43	796641	20.0