LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-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-BF030316.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	5.144	248	250	256	rVB	179093	311093	6.08%	0.746%
2	5.544	282	285	288	rBV	3654508	4169236	81.53%	9.998%
3	6.573	371	375	377	rBV	3685701	4914255	96.10%	11.785%
4	6.710	383	387	389	rBV	3990954	4963772	97.07%	11.903%
5	6.939	404	407	409	rBV	961134	1010388	19.76%	2.423%
6	7.099	418	421	423	rVB	2950176	3746792	73.27%	8.985%
7	7.499	453	456	459	rBV	2369485	3003122	58.73%	7.202%
8	7.579	461	463	466	rBV	40627	60268	1.18%	0.145%
9	8.219	517	519	522	rBV	1369796	1258639	24.61%	3.018%
10	9.305	611	614	616	rBV	4803294	5113838	100.00%	12.263%
11	9.693	646	648	650	rBV	1004663	840911	16.44%	2.017%
12	9.910	664	667	669	rVB	108199	94155	1.84%	0.226%
13	9.979	671	673	675	rVB	1537971	1321531	25.84%	3.169%
14	10.413	707	711	712	rBV	93793	143866	2.81%	0.345%
15	10.630	726	730	733	rBV	47538	83314	1.63%	0.200%
16	10.768	739	742	745	rBV	2345695	2648344	51.79%	6.351%
17	10.882	750	752	757	rVV	160486	181131	3.54%	0.434%
18	11.328	789	791	793	rBV	84546	77174	1.51%	0.185%
19	11.465	801	803	805	rBV	1412806	1206080	23.58%	2.892%
20	11.991	847	849	855	rBV	454688	452179	8.84%	1.084%
21	12.676	907	909	915	rBV	85087	98954	1.94%	0.237%
22	12.779	915	918	925	rVV	165642	250095	4.89%	0.600%
23	12.905	927	929	931	rVV	62594	72497	1.42%	0.174%
24	12.951	931	933	935	rVV	52115	55174	1.08%	0.132%
25	13.054	939	942	945	rBV	3555587	3392861	66.35%	8.136%
26	13.945	1018	1020	1026	rBV	215482	244466	4.78%	0.586%
27	14.105	1030	1034	1036	rBV	1035072	970897	18.99%	2.328%
28	14.574	1073	1075	1078	rBV2	35230	54045	1.06%	0.130%
29	15.145	1122	1125	1129	rBV	25258	52552	1.03%	0.126%
30	15.568	1160	1162	1165	rBV	534550	726881	14.21%	1.743%
31	16.528	1243	1246	1254	rVB6	20674	60584	1.18%	0.145%
32	17.625	1338	1342	1347	rBV5	49040	121619	2.38%	0.292%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

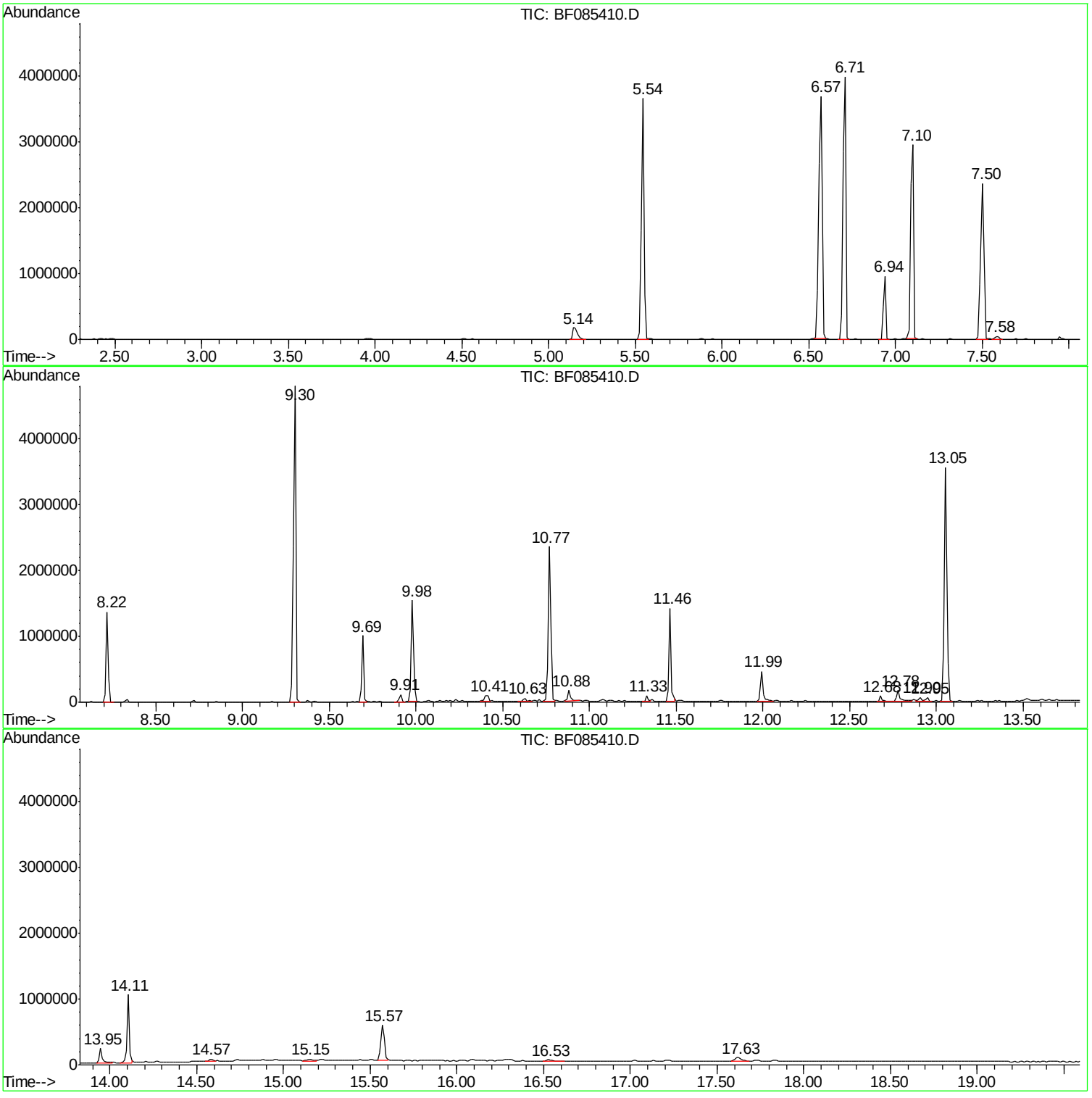
Sum of corrected areas: 41700713

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

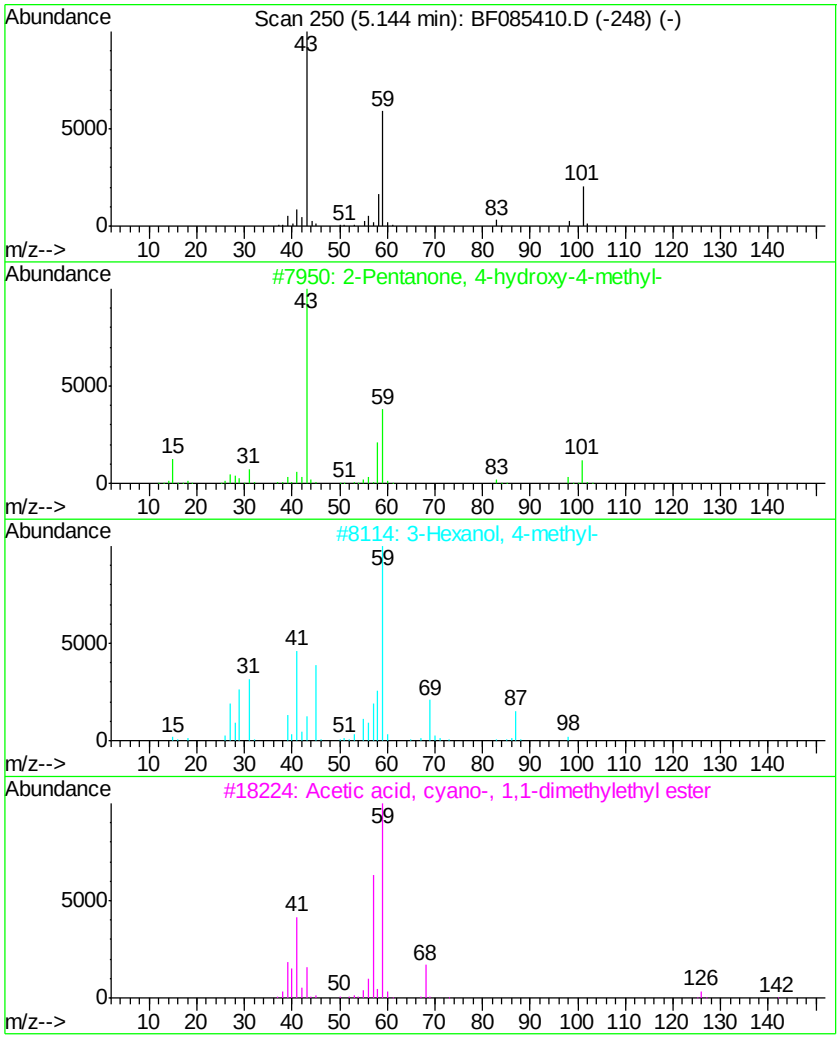
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

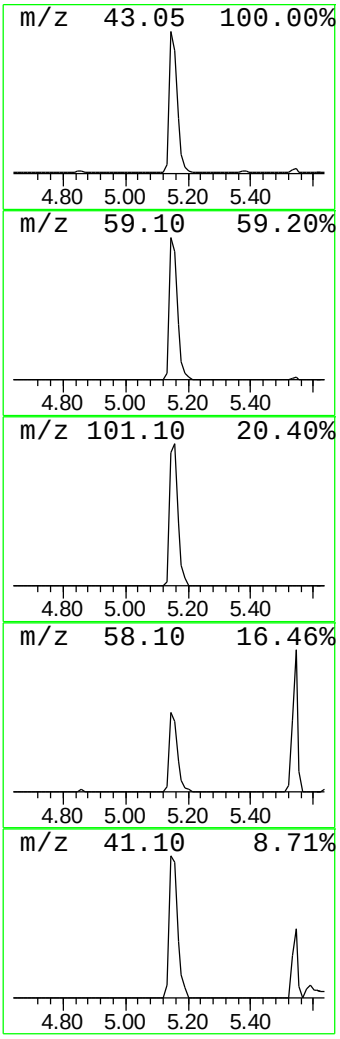
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	6.16 ng	311093	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

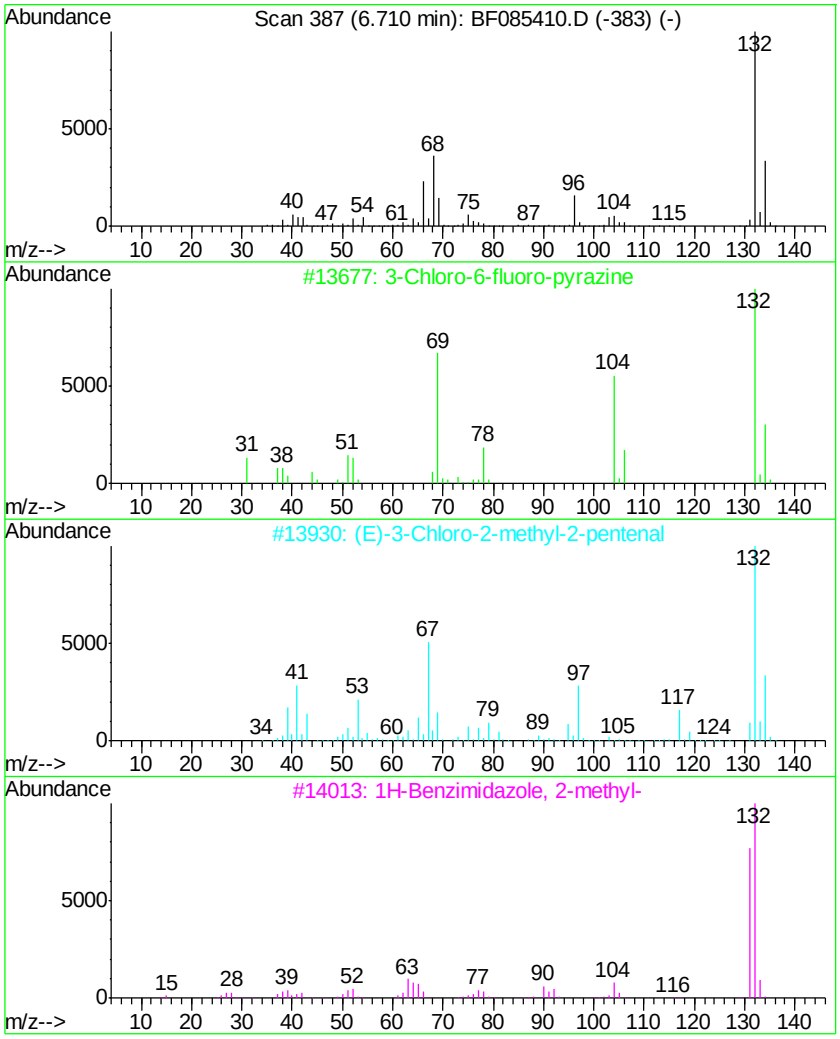
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

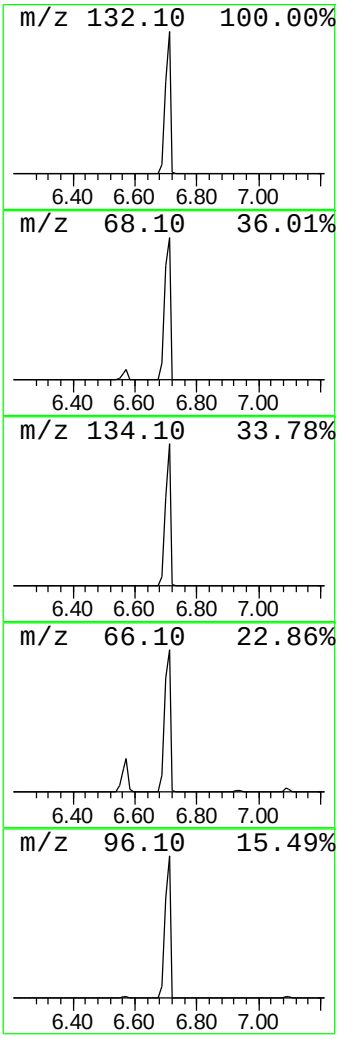
****

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	98.25 ng	4963770	1,4-Dichlorobenzene-d4	6.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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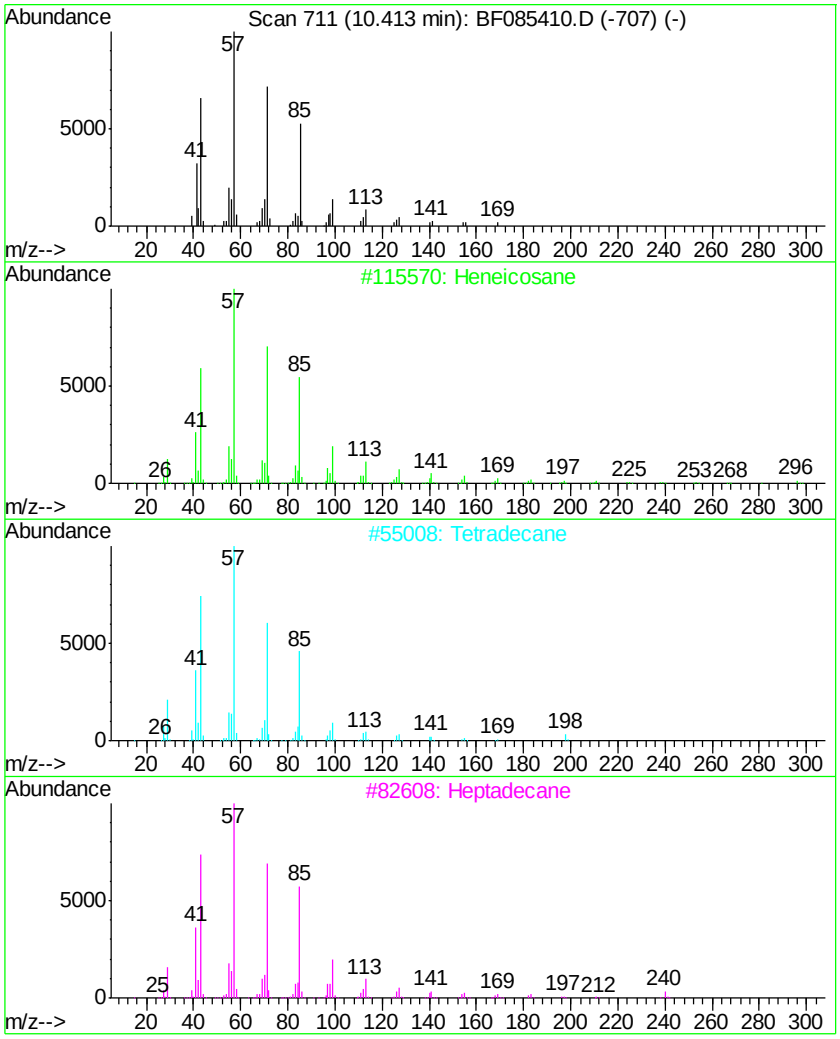
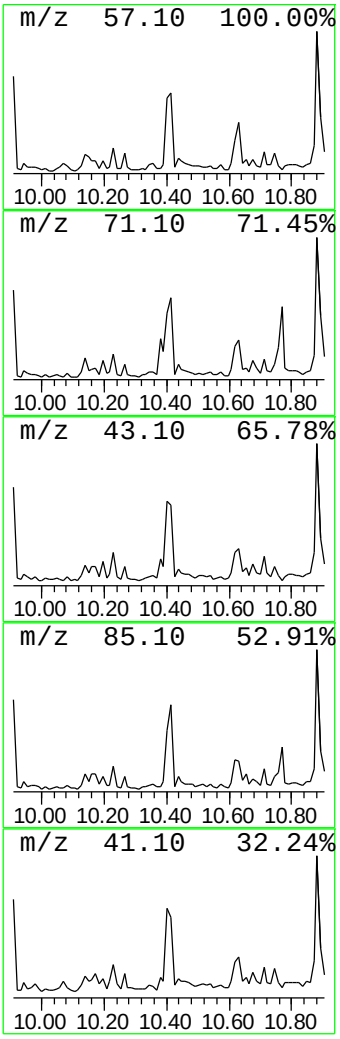
Peak Number 4 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	2.18 ng	143866	Acenaphthene-d10	9.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetradecane	198	C14H30	000629-59-4	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	80
5	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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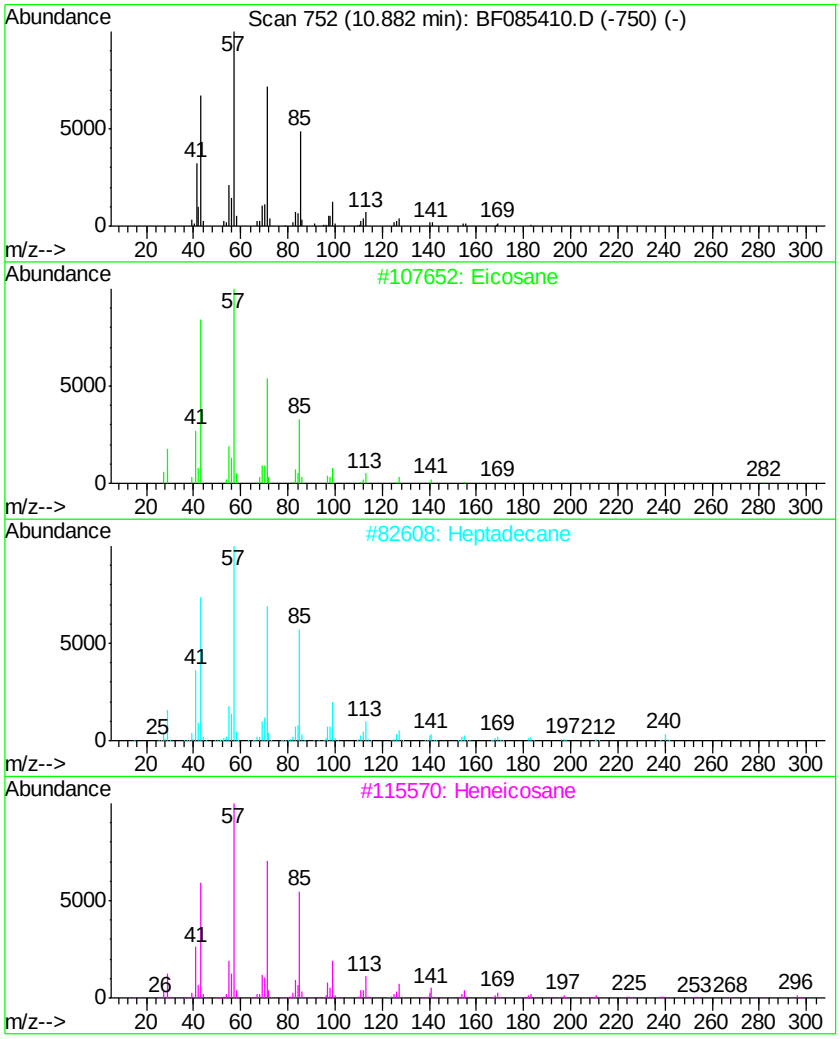
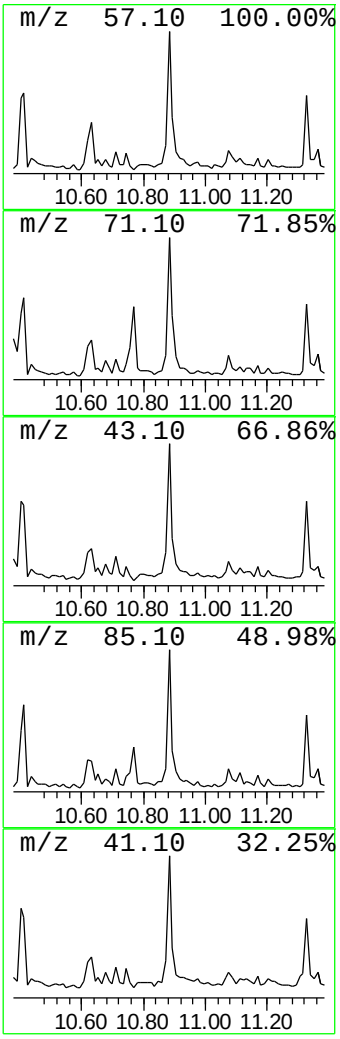
Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	3.00 ng	181131	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Pentadecane	212	C15H32	000629-62-9	90
5	Tetradecane	198	C14H30	000629-59-4	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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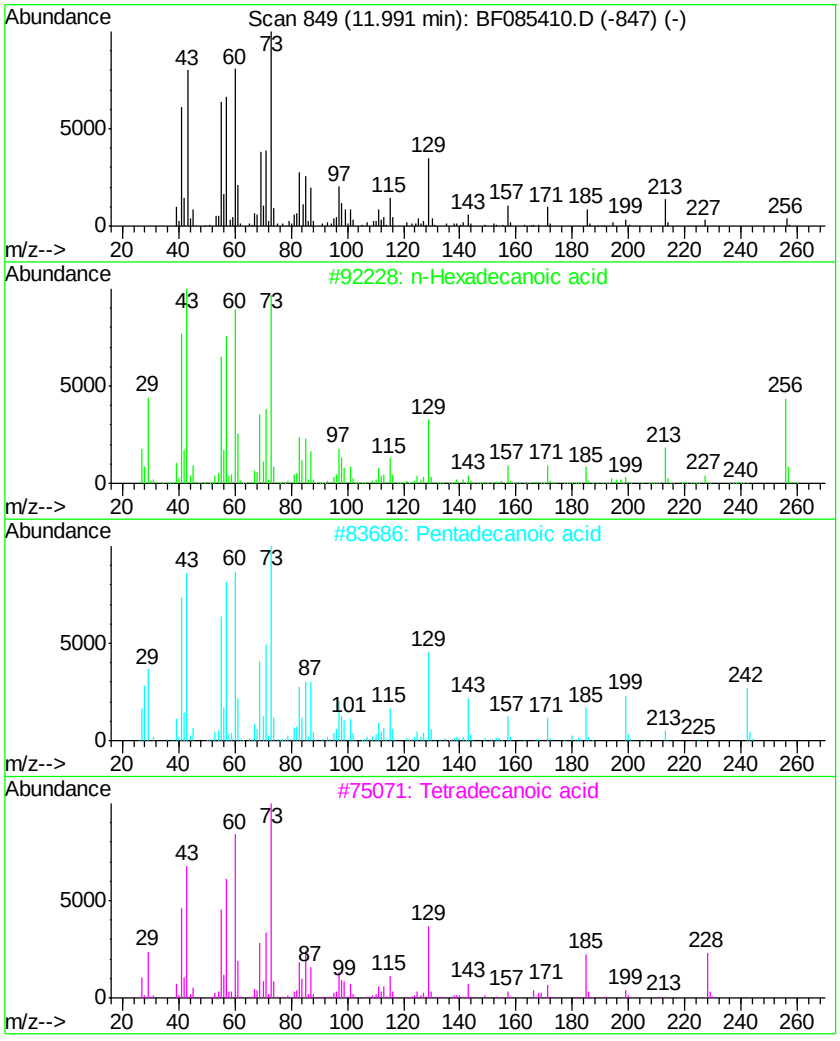
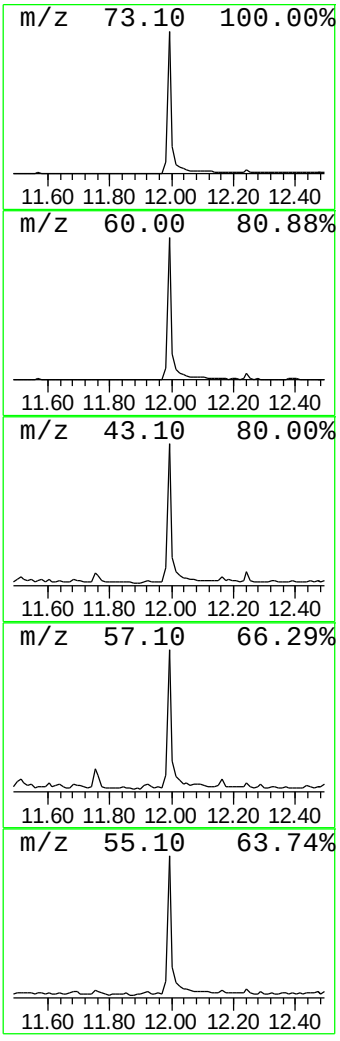
Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	7.50 ng	452179	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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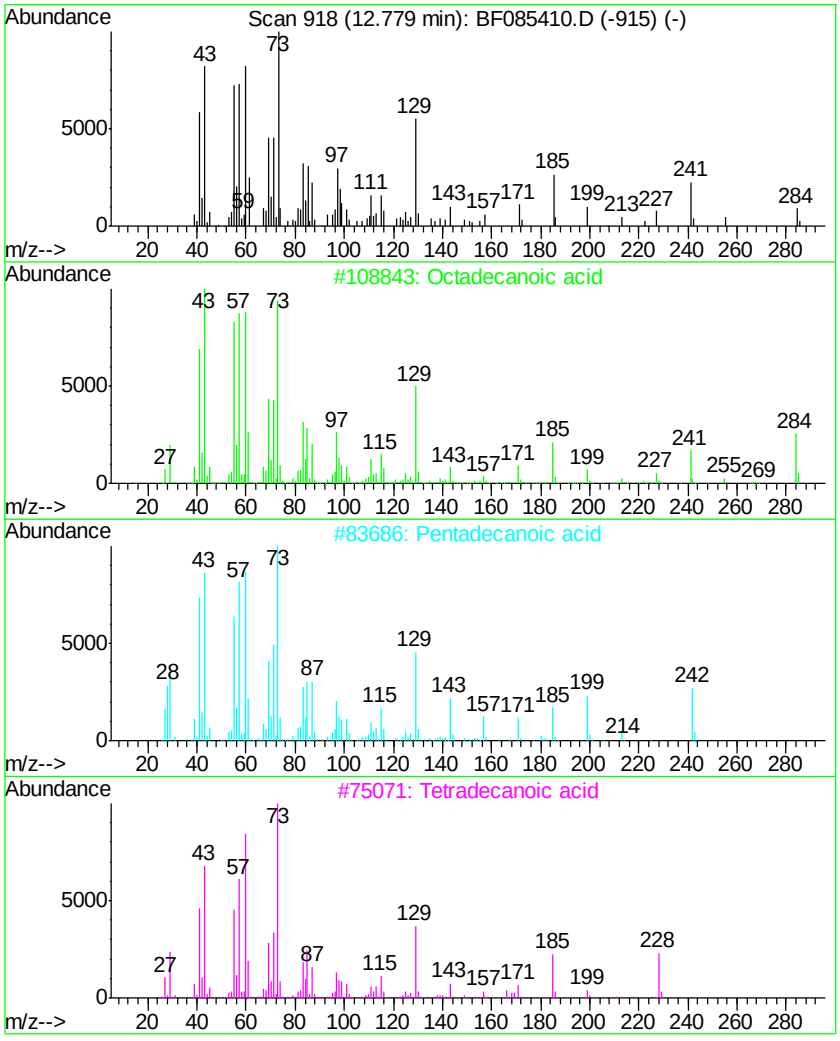
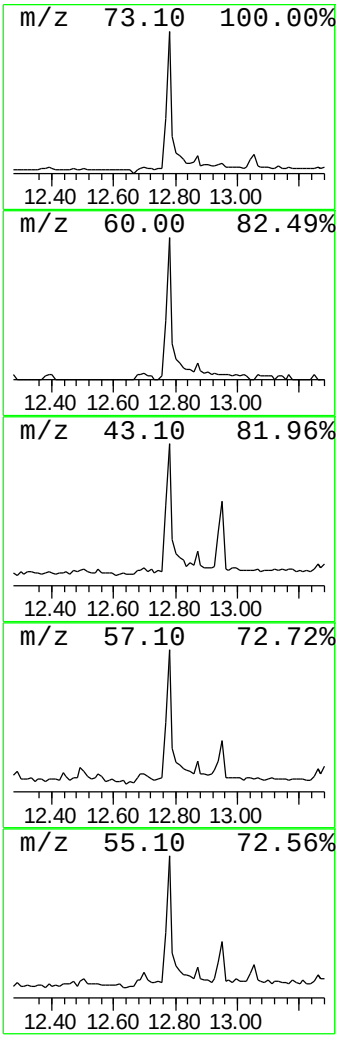
Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	4.15 ng	250095	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

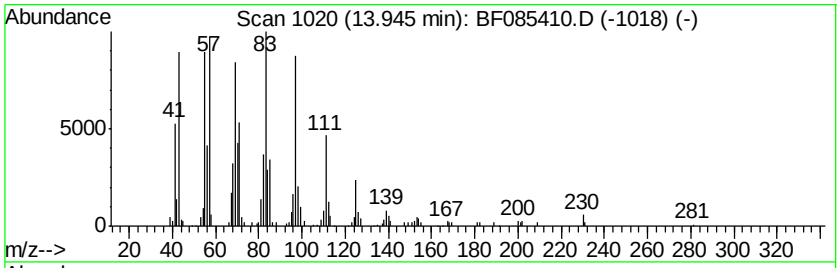
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

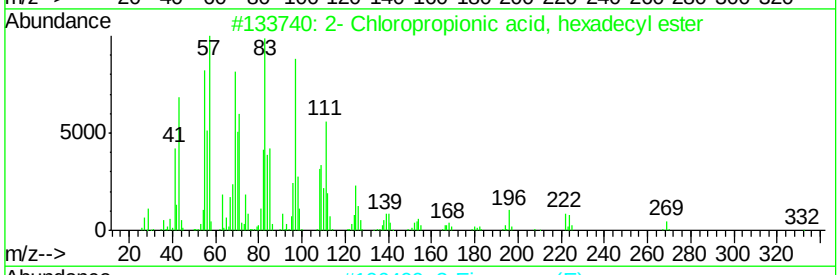
****

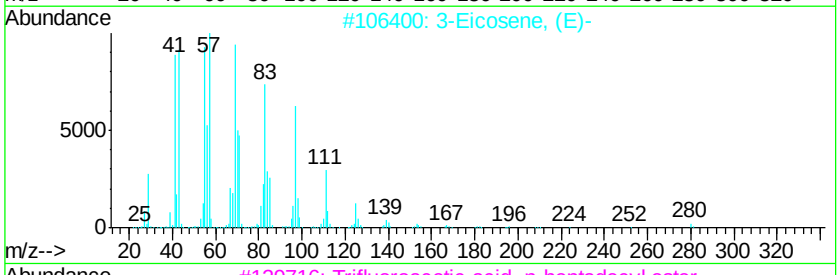
Peak Number 8 2- Chloropropionic acid, he... Concentration Rank 5

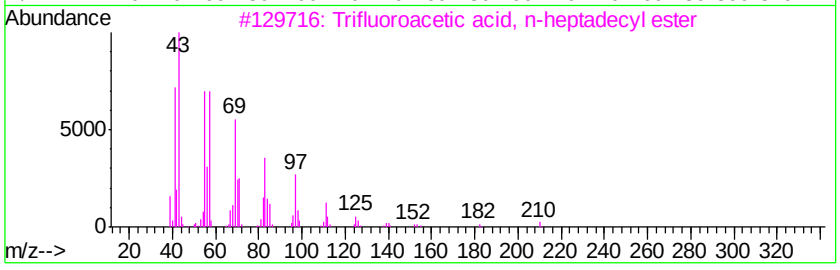
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	5.04 ng	244466	Chrysene-d12	14.11

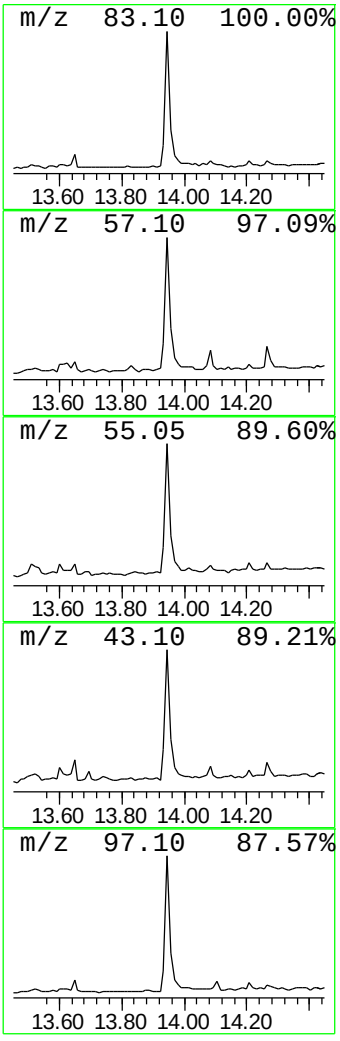
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91











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Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

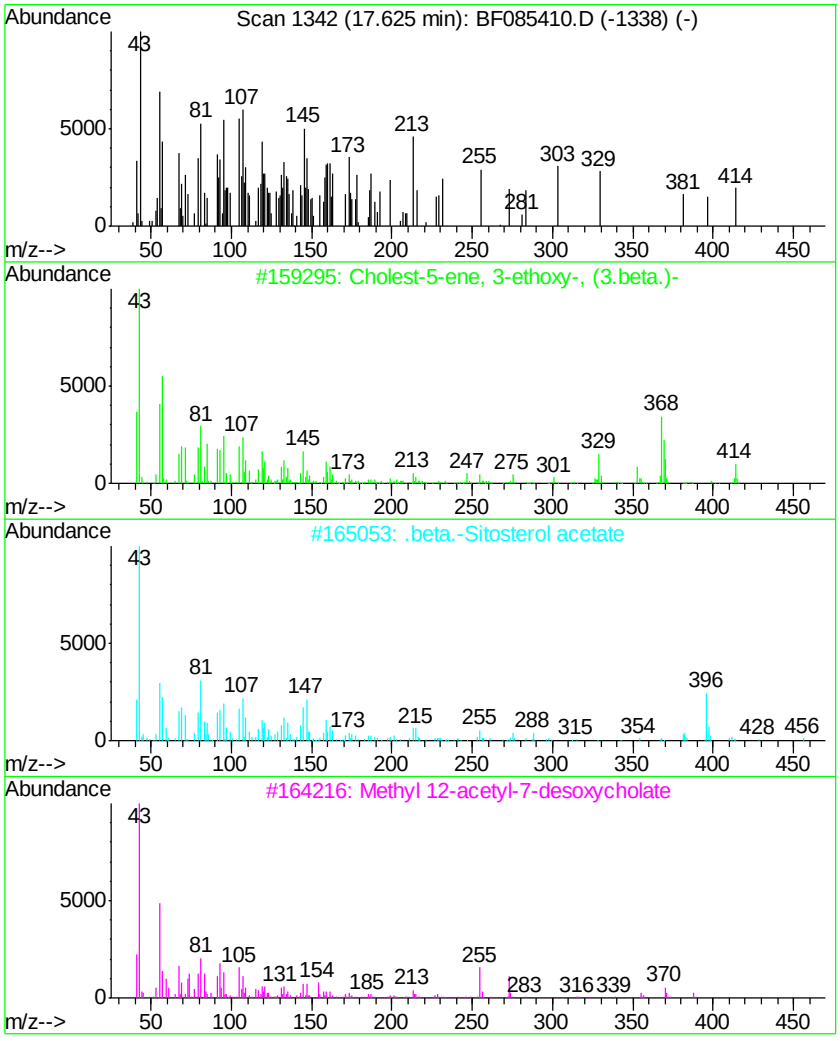
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

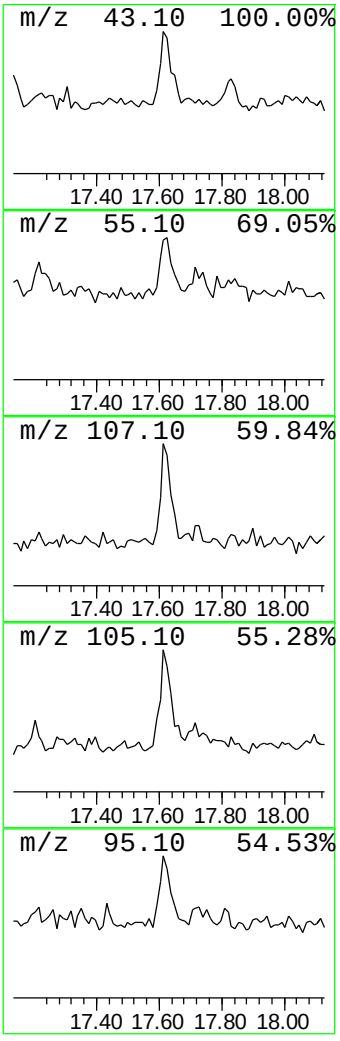
****

Peak Number 9 Cholest-5-ene, 3-ethoxy-, (... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	3.35 ng	121619	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	60
2	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	25
3	Methyl 12-acetyl-7-desoxycholate	448	C27H44O5	055547-48-3	25
4	Clionasterol acetate	456	C31H52O2	004651-54-1	14
5	5-Cholene, 3,24-dihydroxy-	360	C24H40O2	1000251-69-2	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085410.D
Acq On : 12 Mar 2016 10:20
Operator : UM/SJ
Sample : H1731-10
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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...	5.14	6.2	ng	311093	1	6.94	1010390	20.0
unknown6.71	6.71	98.3	ng	4963770	1	6.94	1010390	20.0
Heneicosane	10.41	2.2	ng	143866	3	9.98	1321530	20.0
Eicosane	10.88	3.0	ng	181131	4	11.46	1206080	20.0
n-Hexadecanoic acid	11.99	7.5	ng	452179	4	11.46	1206080	20.0
Octadecanoic acid	12.78	4.2	ng	250095	4	11.46	1206080	20.0
2- Chloropropioni...	13.95	5.0	ng	244466	5	14.11	970897	20.0
Cholest-5-ene, 3-...	17.63	3.4	ng	121619	6	15.57	726881	20.0