LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085411.D
Acq On : 12 Mar 2016 10:48
Operator : UM/SJ
Sample : H1731-12
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-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	247	250	258	rBV	210125	319226	6.89%	0.842%
2	5.544	282	285	288	rBV	3596285	3910073	84.41%	10.318%
3	6.573	372	375	377	rBV	3463724	4615440	99.64%	12.179%
4	6.710	384	387	389	rBV	3643676	4591091	99.11%	12.115%
5	6.939	404	407	409	rBV	872477	903755	19.51%	2.385%
6	7.099	418	421	423	rBV	2716121	3496324	75.48%	9.226%
7	7.499	453	456	459	rBV	2400110	2615074	56.45%	6.900%
8	7.579	461	463	466	rVV	39883	55337	1.19%	0.146%
9	8.219	517	519	522	rBV	1272641	1112156	24.01%	2.935%
10	9.305	611	614	616	rBV	4282988	4632243	100.00%	12.223%
11	9.693	646	648	650	rBV	936134	785591	16.96%	2.073%
12	9.910	664	667	669	rBV	122715	104628	2.26%	0.276%
13	9.979	671	673	675	rVB	1310939	1096677	23.67%	2.894%
14	10.413	707	711	712	rBV	105243	159807	3.45%	0.422%
15	10.631	727	730	731	rBV	53147	76909	1.66%	0.203%
16	10.768	739	742	745	rBV	2170712	2200779	47.51%	5.807%
17	10.882	749	752	758	rVV	159875	190836	4.12%	0.504%
18	11.328	789	791	793	rBV	88473	78291	1.69%	0.207%
19	11.465	801	803	805	rBV	1128458	920988	19.88%	2.430%
20	11.991	847	849	856	rBV	209177	230535	4.98%	0.608%
21	12.779	916	918	923	rBV	47010	77125	1.66%	0.204%
22	13.054	939	942	944	rBV	3372290	3073301	66.35%	8.110%
23	13.945	1018	1020	1027	rBV	617667	689234	14.88%	1.819%
24	14.105	1032	1034	1036	rVV	928951	798421	17.24%	2.107%
25	14.574	1073	1075	1082	rBV	53749	113644	2.45%	0.300%
26	14.951	1106	1108	1111	rVB	140600	177258	3.83%	0.468%
27	15.568	1159	1162	1165	rBV	506792	664427	14.34%	1.753%
28	16.083	1205	1207	1212	rBV	60053	133400	2.88%	0.352%
29	17.626	1338	1342	1348	rVB6	27233	74411	1.61%	0.196%

Sum of corrected areas: 37896981

LSC Report - Integrated Chromatogram

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Misc :
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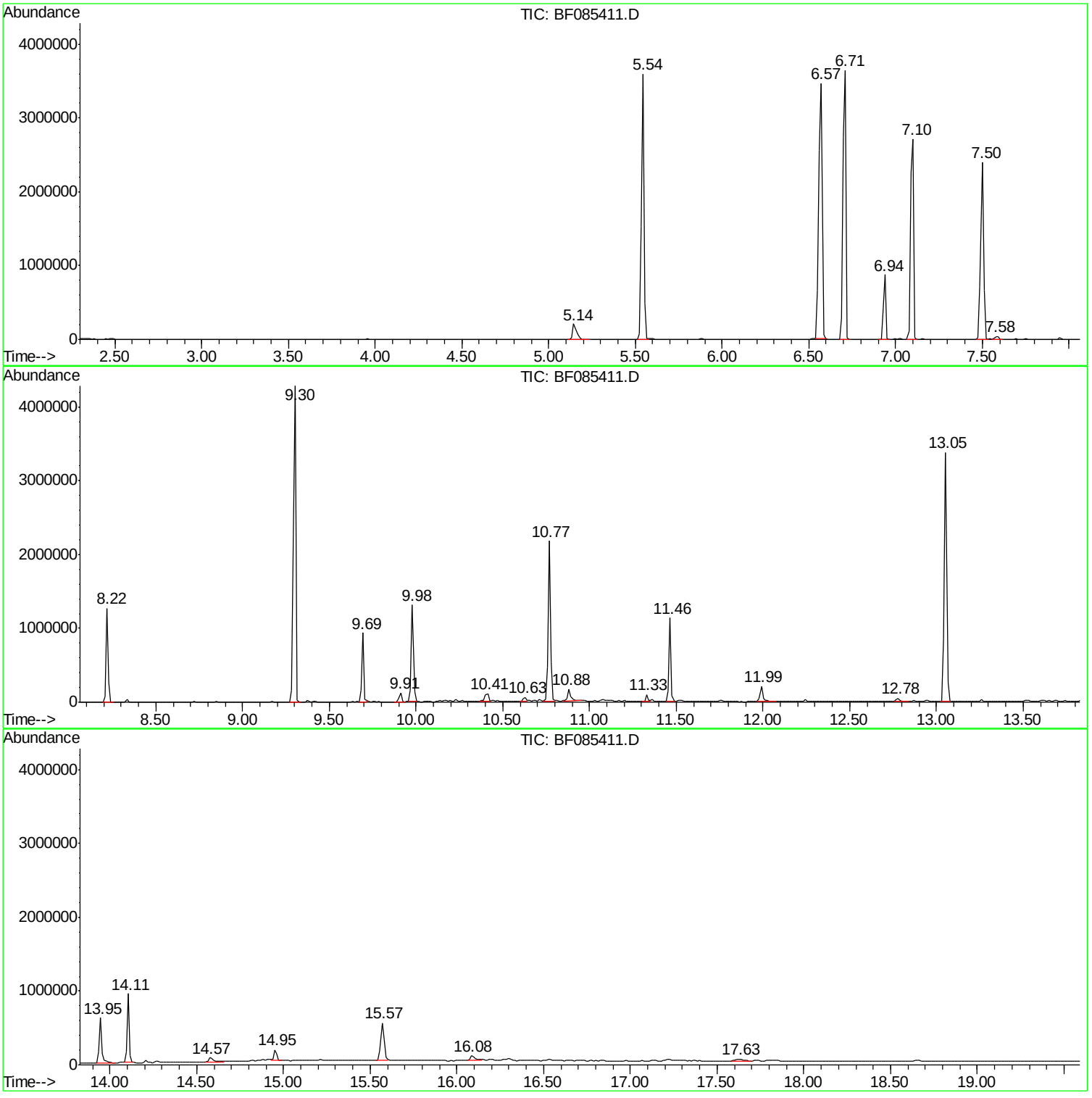
Instrument : BNA_F
ClientSampleId : SB-28-COMP

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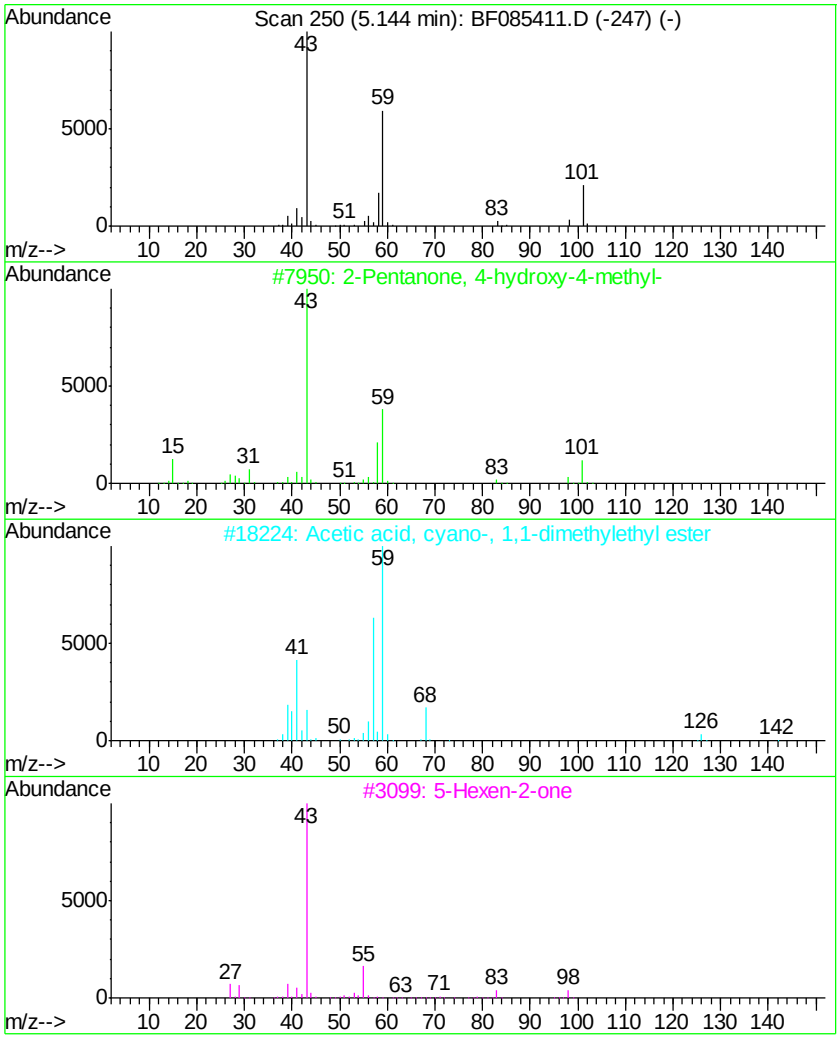
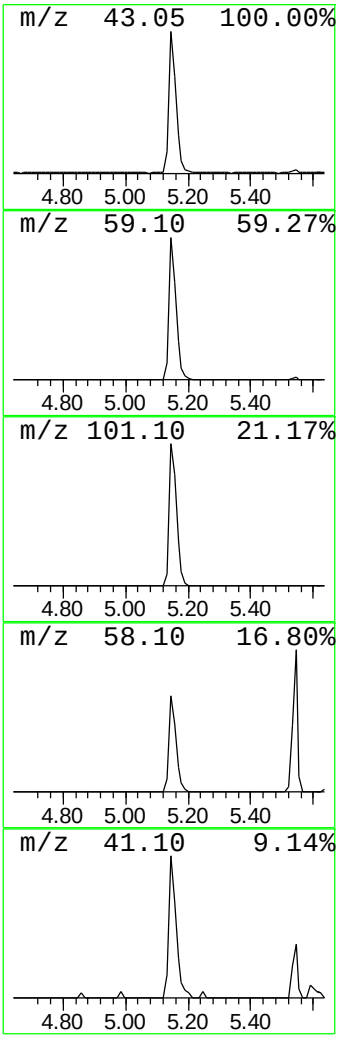
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	7.06 ng	319226	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

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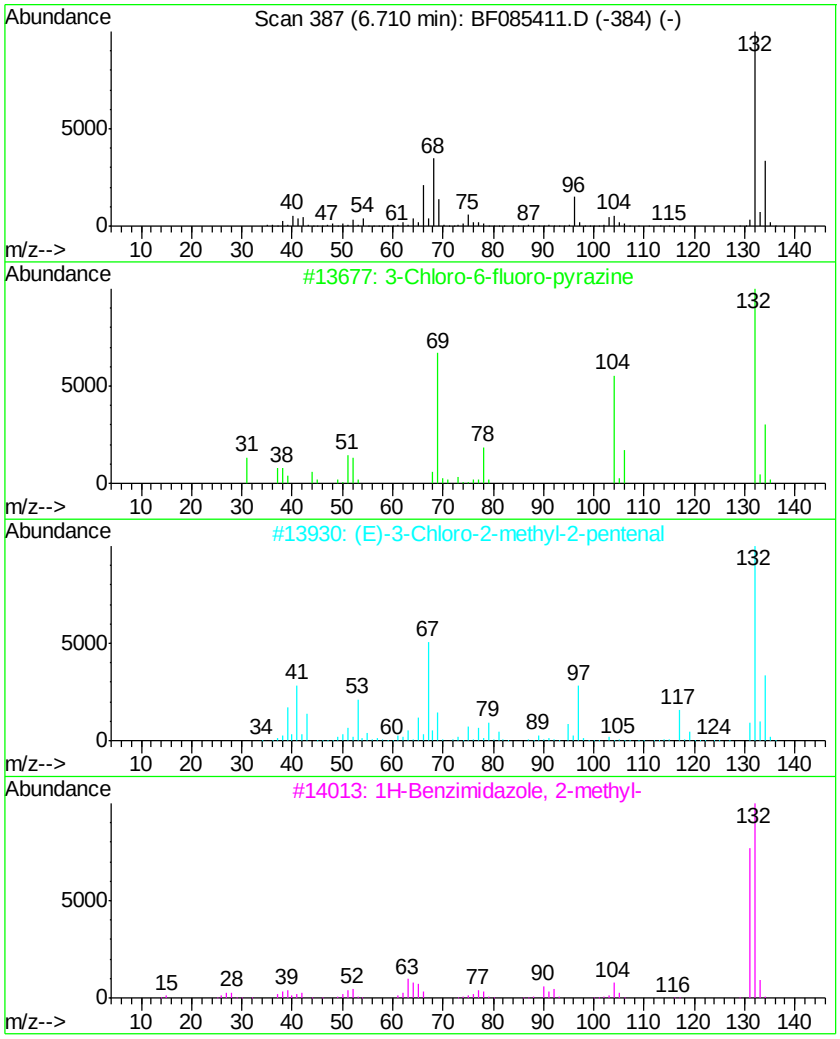
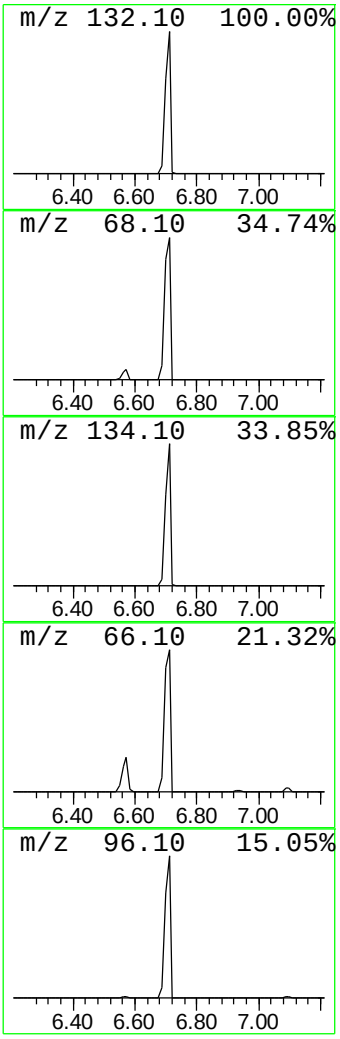
Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	101.60 ng	4591090	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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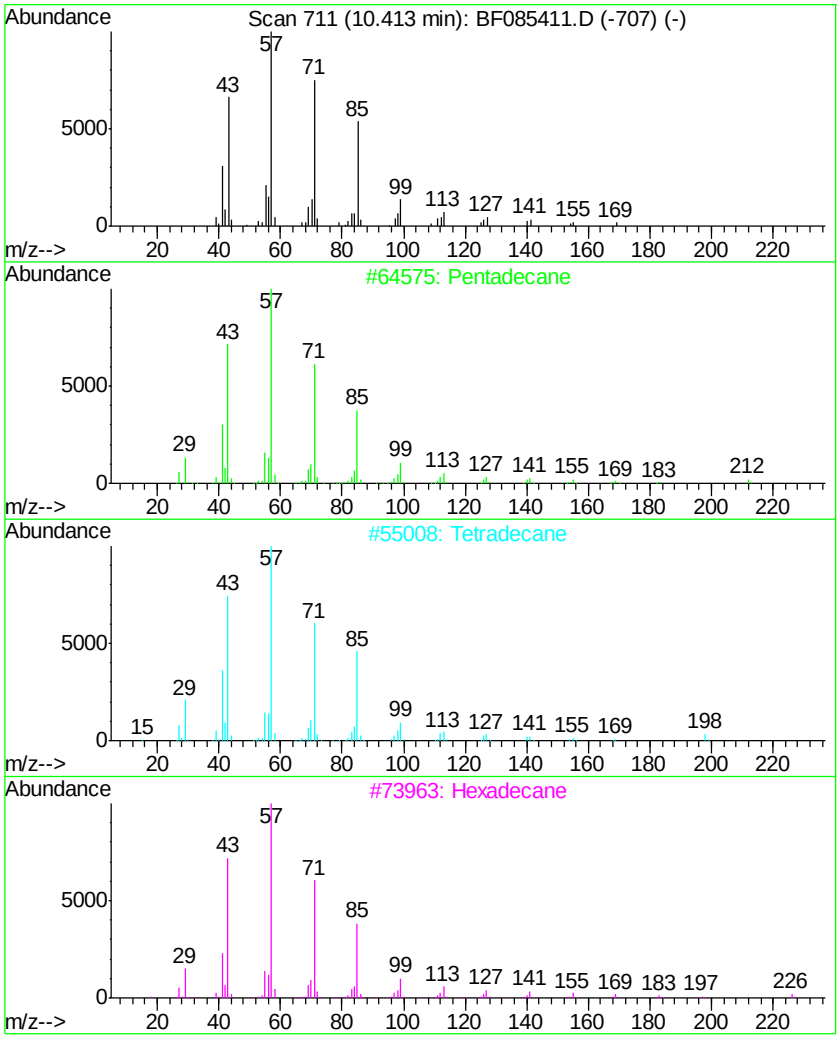
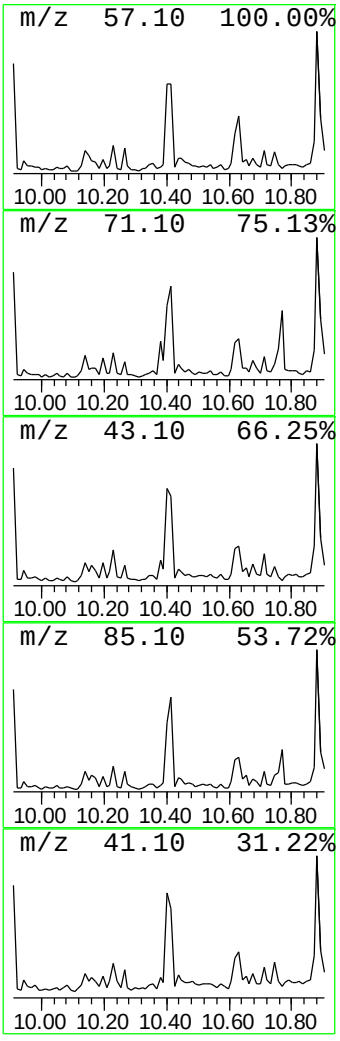
****

Peak Number 4 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	2.91 ng	159807	Acenaphthene-d10	9.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Tetradecane	198	C14H30	000629-59-4	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane	240	C17H36	000629-78-7	83
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80





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Instrument : BNA_F
ClientSampleId : SB-28-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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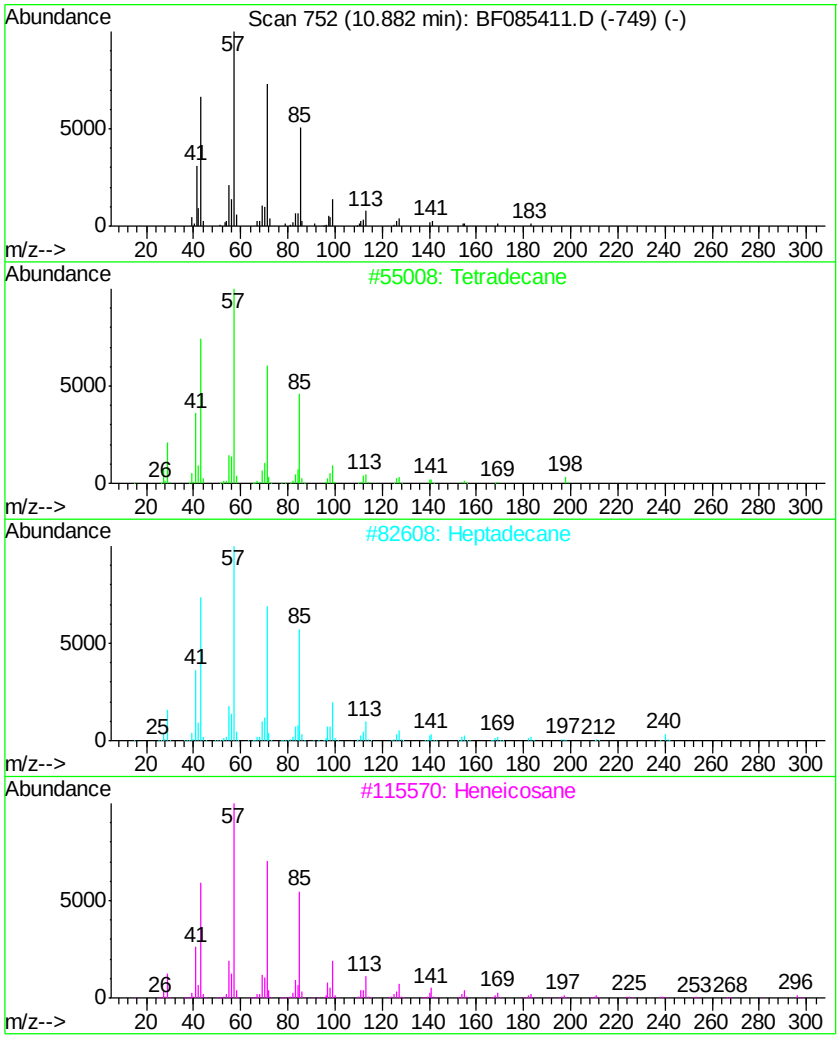
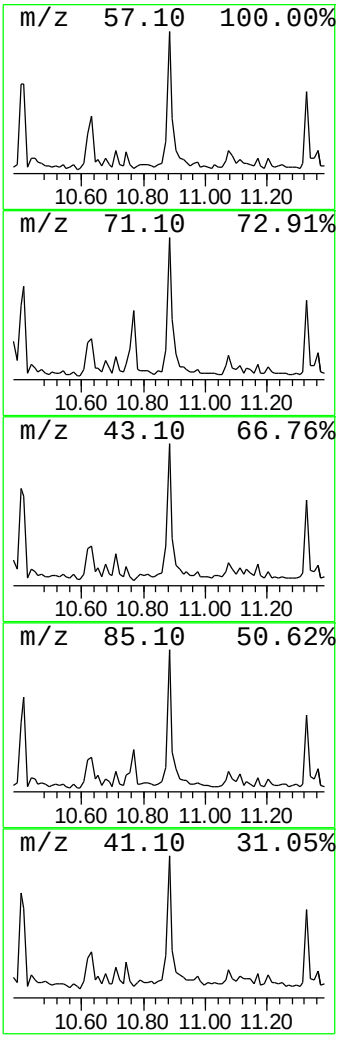
Peak Number 5 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	4.14 ng	190836	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentadecane	212	C15H32	000629-62-9	90
5	Hexadecane	226	C16H34	000544-76-3	90





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ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
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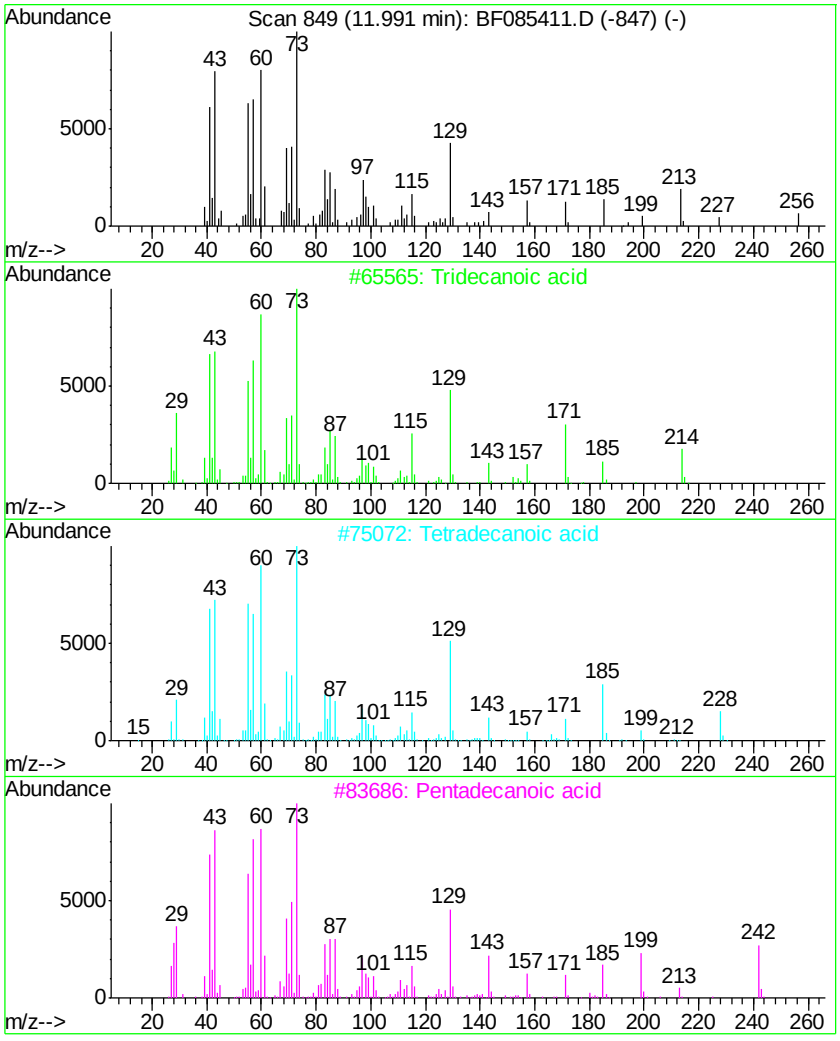
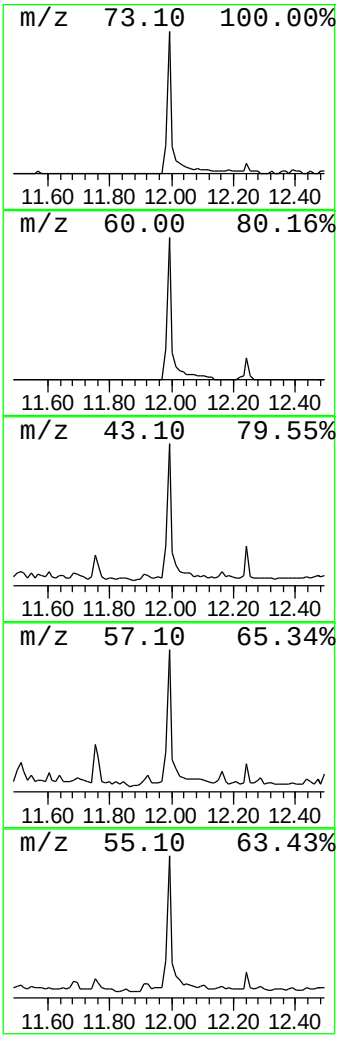
Peak Number 6 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	5.01 ng	230535	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62





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Instrument : BNA_F
ClientSampleId : SB-28-COMP

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TIC Library : C:\DATABASE\NIST02.L
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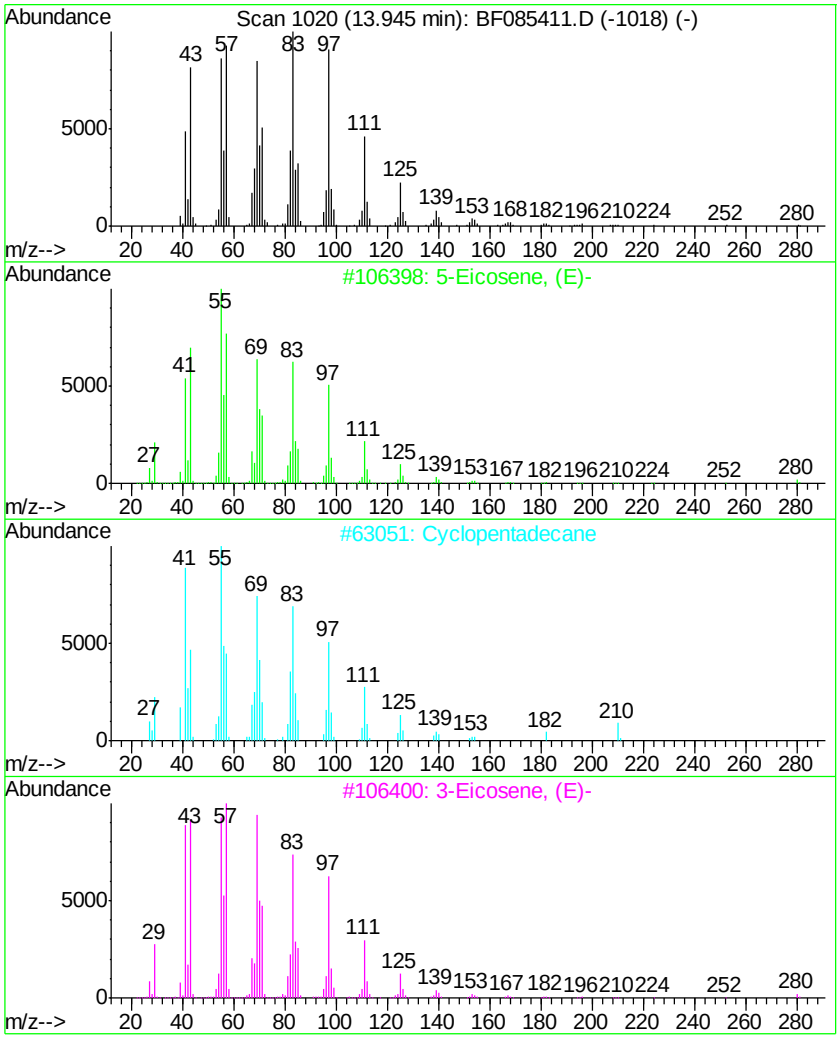
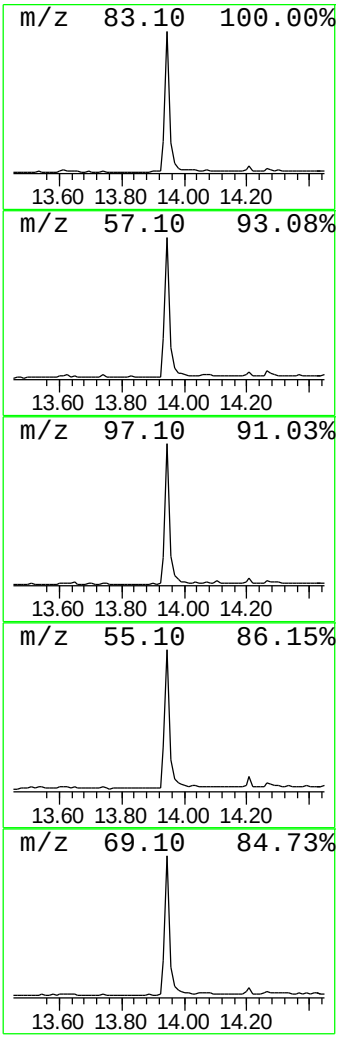
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	17.26 ng	689234	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





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

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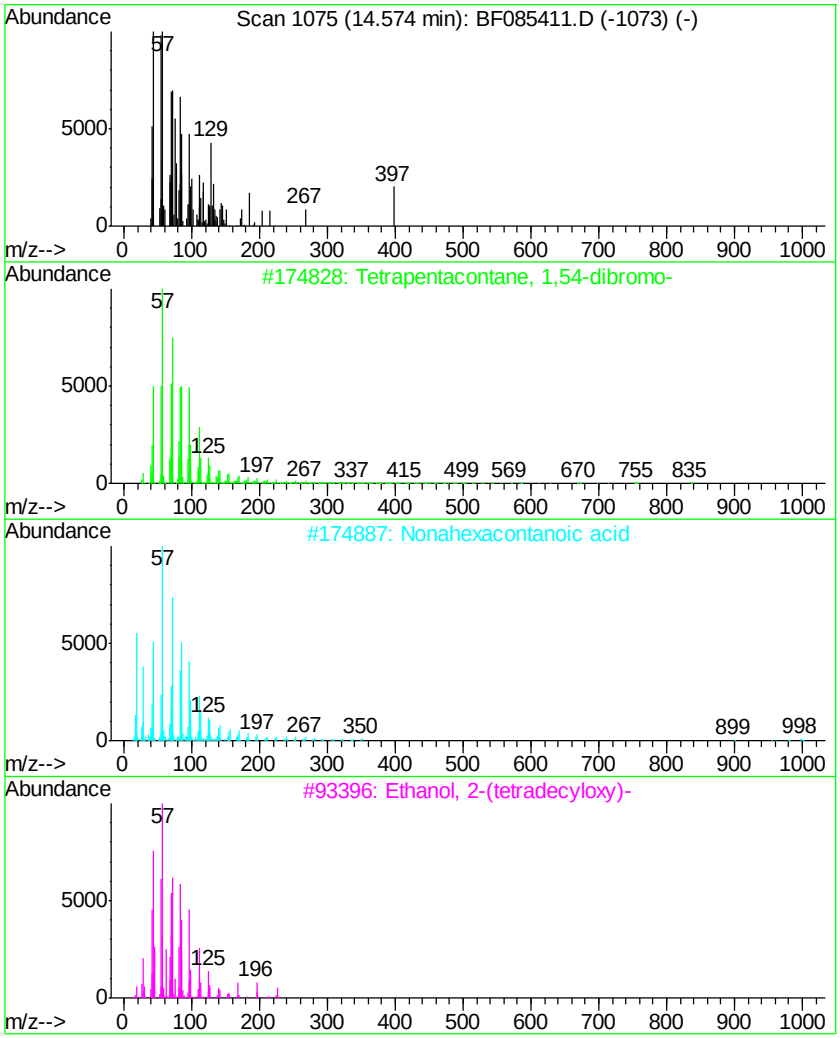
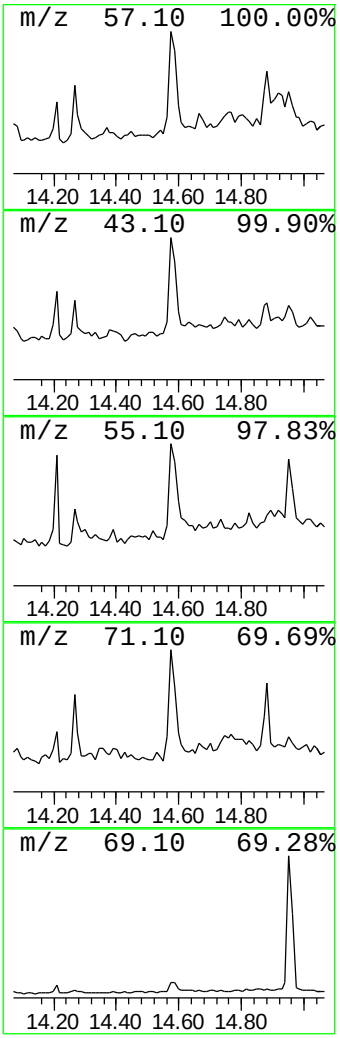
Peak Number 8 Tetrapentacontane, 1,54-dib... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.85 ng	113644	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	50
2	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	43
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	41
4	Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	41
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	38





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TIC Library : C:\DATABASE\NIST02.L
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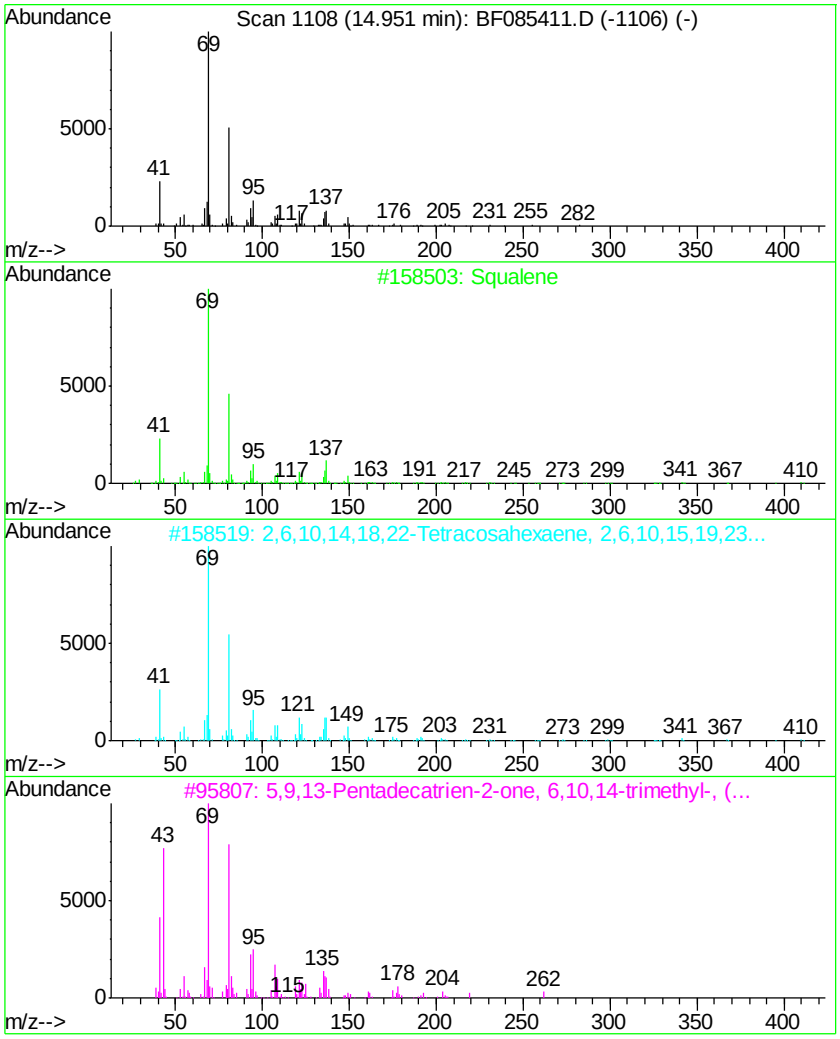
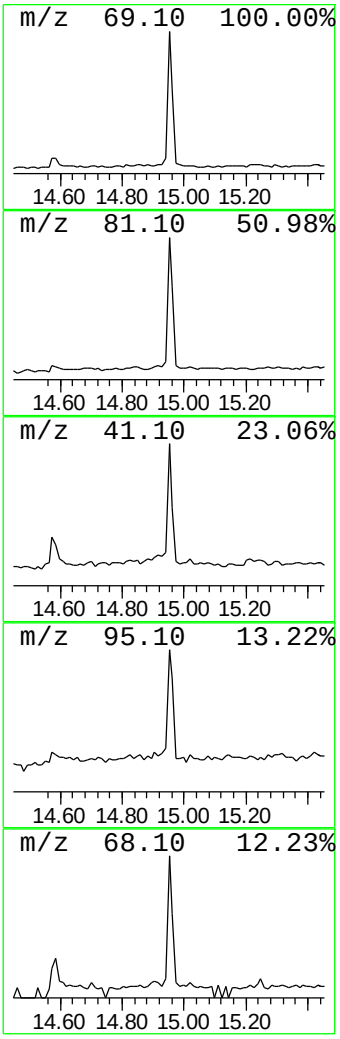
Peak Number 9 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	5.34 ng	177258	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	64





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

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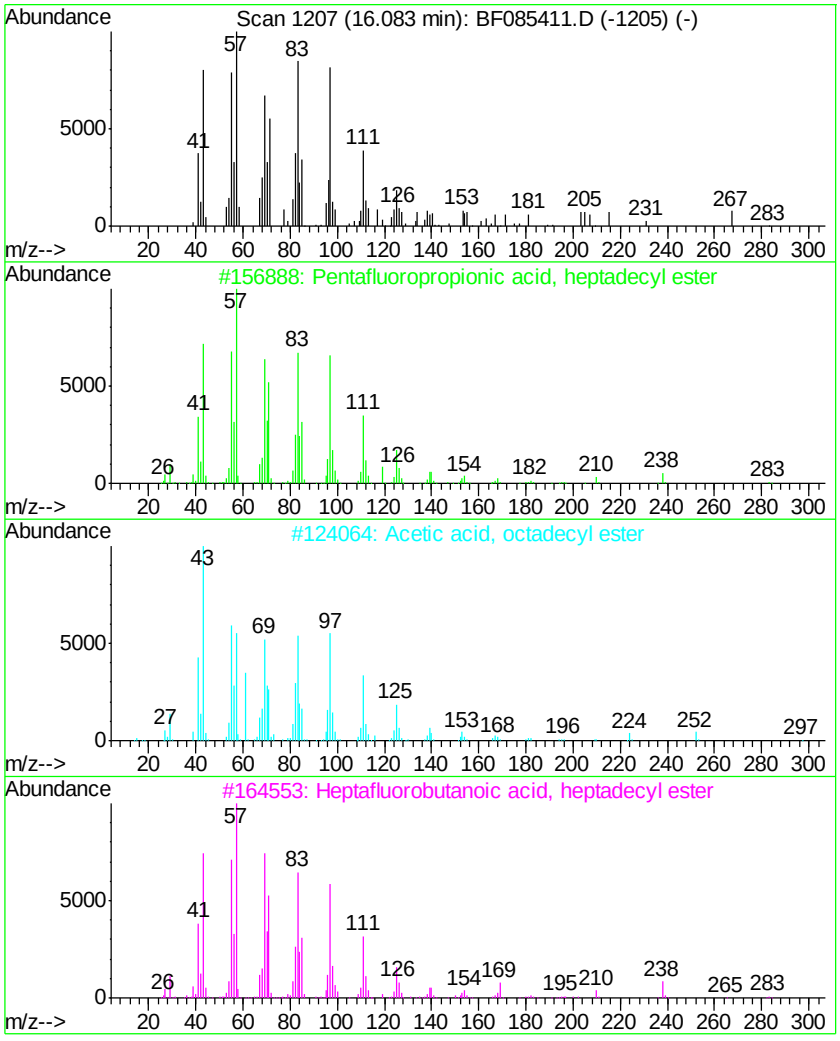
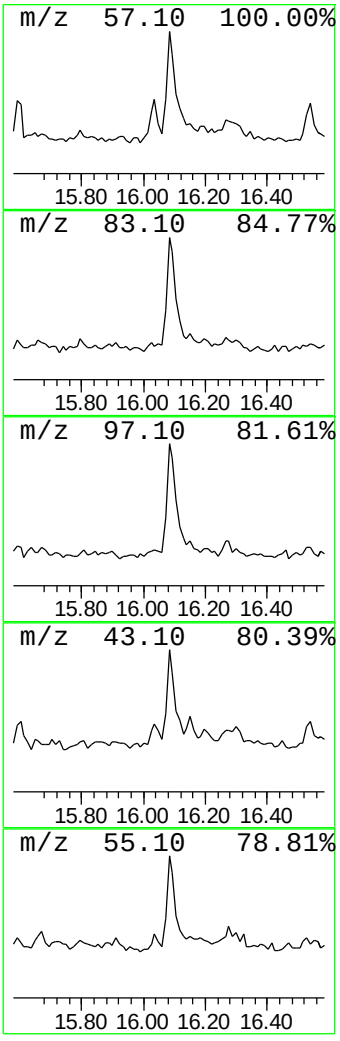
Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	4.02 ng	133400	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
2	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	83
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81
4	17-Pentatriacontene	491	C35H70	006971-40-0	74
5	1-Hexacosanol	382	C26H54O	000506-52-5	58





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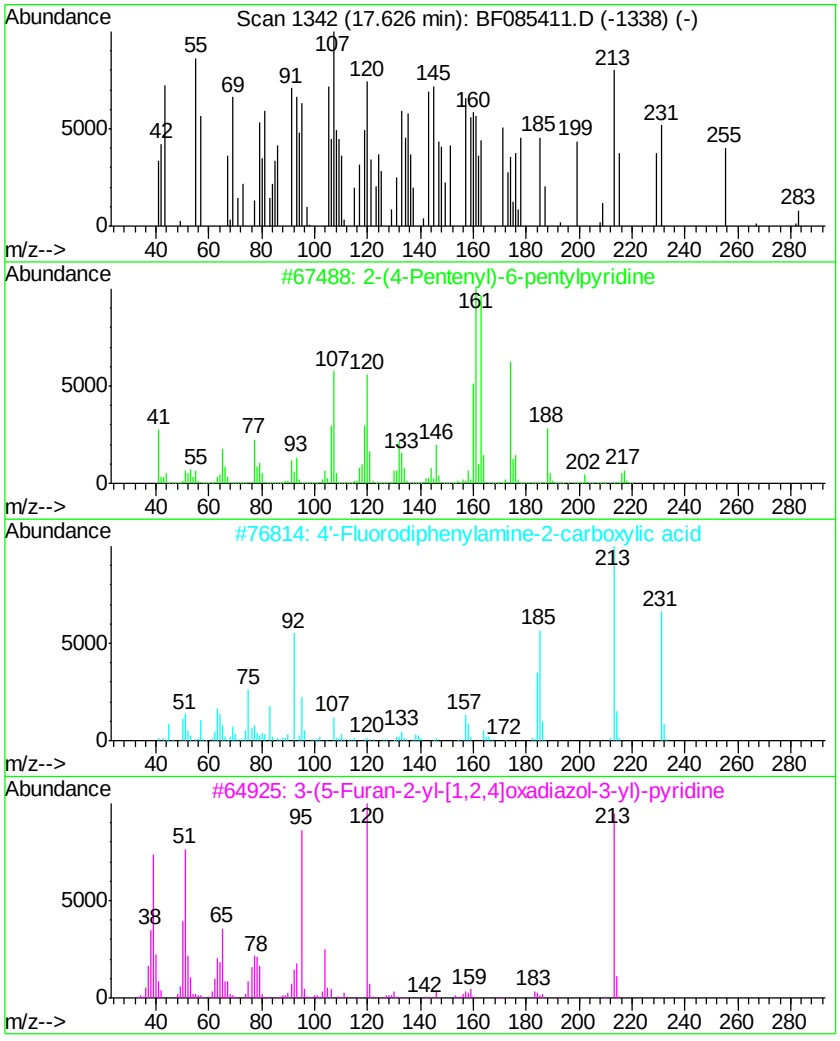
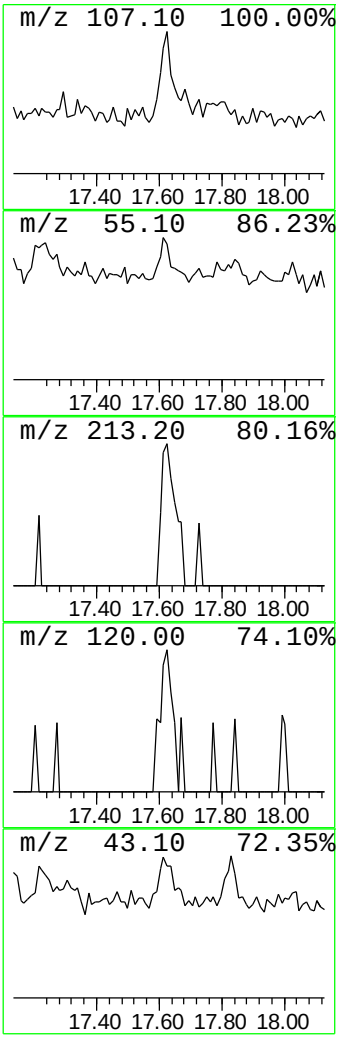
****

Peak Number 11 unknown17.63 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.63	2.24 ng	74411	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Pentenyl)-6-pentylpyridine	217	C15H23N	1000111-47-8	22
2	4'-Fluorodiphenylamine-2-carboxy...	231	C13H10FNO2	000054-60-4	14
3	3-(5-Furan-2-yl-[1,2,4]oxadiazol...	213	C11H7N3O2	1000277-85-7	14
4	Benzamide, 4-acetylamino-	178	C9H10N2O2	058202-83-8	11
5	Pyrido[4,3-d]pyrimidine-2,4(1H,3...	163	C7H5N3O2	016952-65-1	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085411.D
Acq On : 12 Mar 2016 10:48
Operator : UM/SJ
Sample : H1731-12
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-28-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	7.1	ng	319226	1	6.94	903755	20.0
unknown6.71	6.71	101.6	ng	4591090	1	6.94	903755	20.0
Pentadecane	10.41	2.9	ng	159807	3	9.98	1096680	20.0
Tetradecane	10.88	4.1	ng	190836	4	11.46	920988	20.0
Tridecanoic acid	11.99	5.0	ng	230535	4	11.46	920988	20.0
5-Eicosene, (E)-	13.95	17.3	ng	689234	5	14.11	798421	20.0
Tetrapentacontane...	14.57	2.9	ng	113644	5	14.11	798421	20.0
Squalene	14.95	5.3	ng	177258	6	15.57	664427	20.0
Pentafluoropropio...	16.08	4.0	ng	133400	6	15.57	664427	20.0
unknown17.63	17.63	2.2	ng	74411	6	15.57	664427	20.0