LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086900.D
Acq On : 11 May 2016 21:05
Operator : UM/SJ
Sample : H2894-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP18-8FT

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-BF050916.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	1.632	3	4	12	rVB	1121670	1700042	29.76%	2.551%
2	1.747	12	14	19	rBV	3665638	5297031	92.72%	7.947%
3	4.787	278	280	291	rBV	401496	769609	13.47%	1.155%
4	5.233	316	319	321	rBV	4170480	5407875	94.66%	8.114%
5	5.633	352	354	361	rVB	55136	81110	1.42%	0.122%
6	6.296	409	412	419	rBV	4475490	5403695	94.59%	8.107%
7	6.410	419	422	424	rBV	3809295	5453290	95.45%	8.182%
8	6.627	439	441	448	rVB	2060132	1993060	34.89%	2.990%
9	6.787	452	455	457	rBV	4187847	4071402	71.27%	6.108%
10	7.210	488	492	494	rBV	2636951	3899969	68.27%	5.851%
11	7.919	551	554	556	rBV	2665921	2625669	45.96%	3.939%
12	9.005	645	649	651	rBV	3965549	5712978	100.00%	8.571%
13	9.393	681	683	686	rBV	375738	485287	8.49%	0.728%
14	9.610	700	702	704	rBV	161023	140064	2.45%	0.210%
15	9.668	704	707	709	rBV	3073476	2873102	50.29%	4.311%
16	9.839	719	722	724	rBV	32015	64514	1.13%	0.097%
17	10.113	743	746	747	rVV	262579	247299	4.33%	0.371%
18	10.330	762	765	768	rBV	108547	168986	2.96%	0.254%
19	10.456	773	776	779	rBV	3498804	3717503	65.07%	5.577%
20	10.582	784	787	791	rVV	364446	431347	7.55%	0.647%
21	10.708	796	798	800	rVV	77975	93152	1.63%	0.140%
22	10.776	801	804	808	rVB	45601	101530	1.78%	0.152%
23	10.936	814	818	820	rBV3	59313	98663	1.73%	0.148%
24	11.028	824	826	827	rVV	259574	222553	3.90%	0.334%
25	11.051	827	828	831	rVV	57155	70425	1.23%	0.106%
26	11.142	834	836	839	rVV	2751019	2661411	46.59%	3.993%
27	11.199	839	841	846	rVB2	35922	66501	1.16%	0.100%
28	11.451	861	863	865	rBV	150712	121888	2.13%	0.183%
29	11.702	882	885	891	rBV2	343568	618616	10.83%	0.928%
30	11.851	897	898	900	rBV	67283	87015	1.52%	0.131%
31	12.239	930	932	935	rVB	77036	83692	1.46%	0.126%
32	12.479	950	953	955	rVV	111415	162314	2.84%	0.244%
33	12.559	959	960	963	rVV	65904	70030	1.23%	0.105%
34	12.616	963	965	966	rVV	84544	80508	1.41%	0.121%

LSC Area Percent Report

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Data File : BF086900.D
Acq On : 11 May 2016 21:05
Operator : UM/SJ
Sample : H2894-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP18-8FT

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-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.639	966	967	969	rVB	119326	87936	1.54%	0.132%
36	12.731	972	975	978	rBV	4615572	4799058	84.00%	7.200%
37	12.971	993	996	998	rBV	95336	94548	1.65%	0.142%
38	13.314	1023	1026	1030	rBV3	69127	143051	2.50%	0.215%
39	13.645	1052	1055	1063	rBV	204000	573426	10.04%	0.860%
40	13.771	1063	1066	1068	rBV	2616971	2531056	44.30%	3.797%
41	13.954	1079	1082	1084	rBV	70782	74937	1.31%	0.112%
42	14.251	1106	1108	1110	rBV	58175	78447	1.37%	0.118%
43	14.525	1130	1132	1137	rBV2	138454	266188	4.66%	0.399%
44	14.845	1158	1160	1162	rBV	66605	75064	1.31%	0.113%
45	15.131	1182	1185	1187	rBV	1640519	1952117	34.17%	2.929%
46	15.165	1187	1188	1191	rVB	88603	93202	1.63%	0.140%
47	15.531	1218	1220	1224	rVB	82535	118026	2.07%	0.177%
48	15.645	1224	1230	1233	rBV4	21863	84021	1.47%	0.126%
49	15.954	1254	1257	1264	rVB	88289	157203	2.75%	0.236%
50	16.445	1297	1300	1307	rBV	65408	132850	2.33%	0.199%
51	17.028	1347	1351	1358	rVB	53216	136611	2.39%	0.205%
52	17.714	1405	1411	1418	rBV	31579	97735	1.71%	0.147%
53	18.526	1477	1482	1490	rBV	22940	74863	1.31%	0.112%

Sum of corrected areas: 66652469

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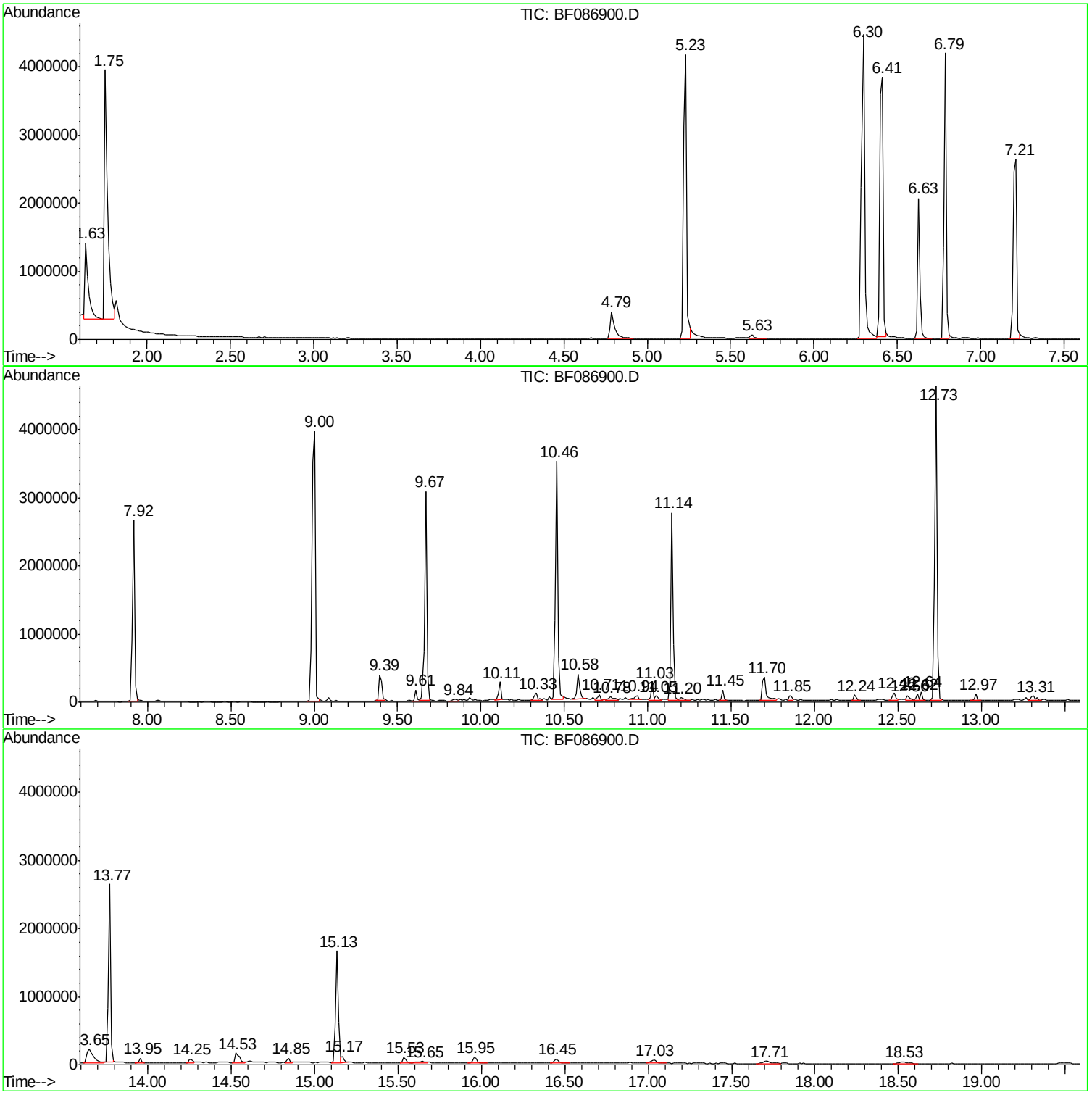
Operator : UM/SJ
Sample : H2894-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP18-8FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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\BF051116\
Data File : BF086900.D
Acq On : 11 May 2016 21:05
Operator : UM/SJ
Sample : H2894-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP18-8FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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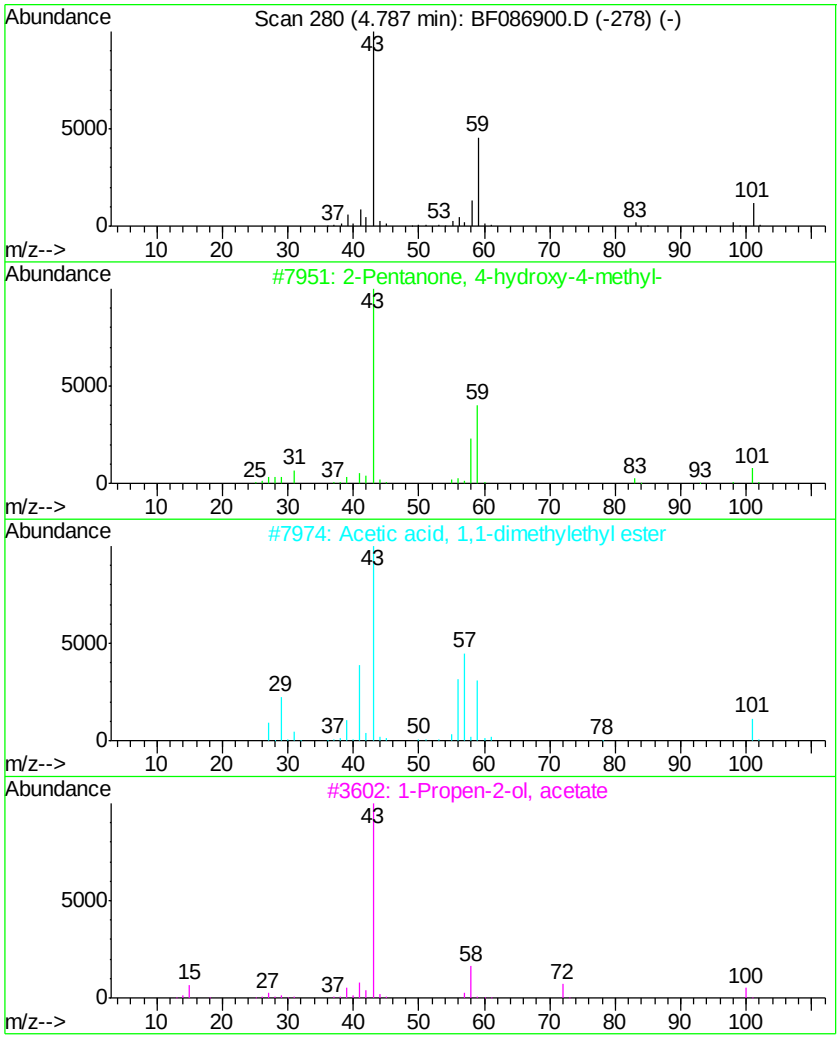
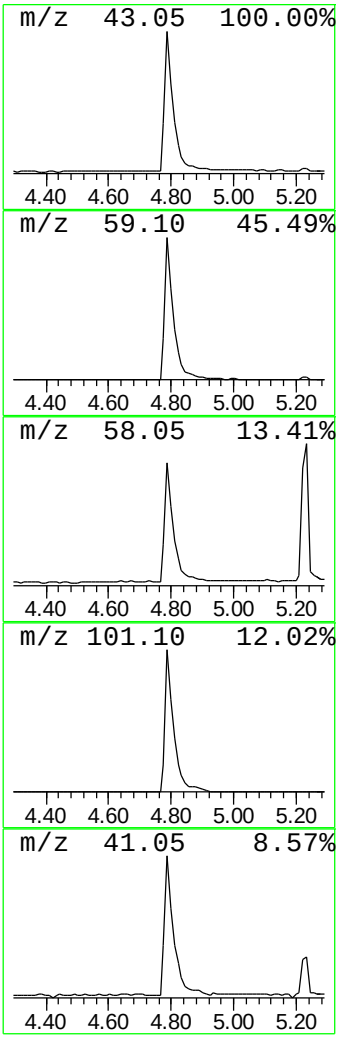
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	7.72 ng	769609	1,4-Dichlorobenzene-d4	6.63

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9





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Acq On : 11 May 2016 21:05
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Sample : H2894-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP18-8FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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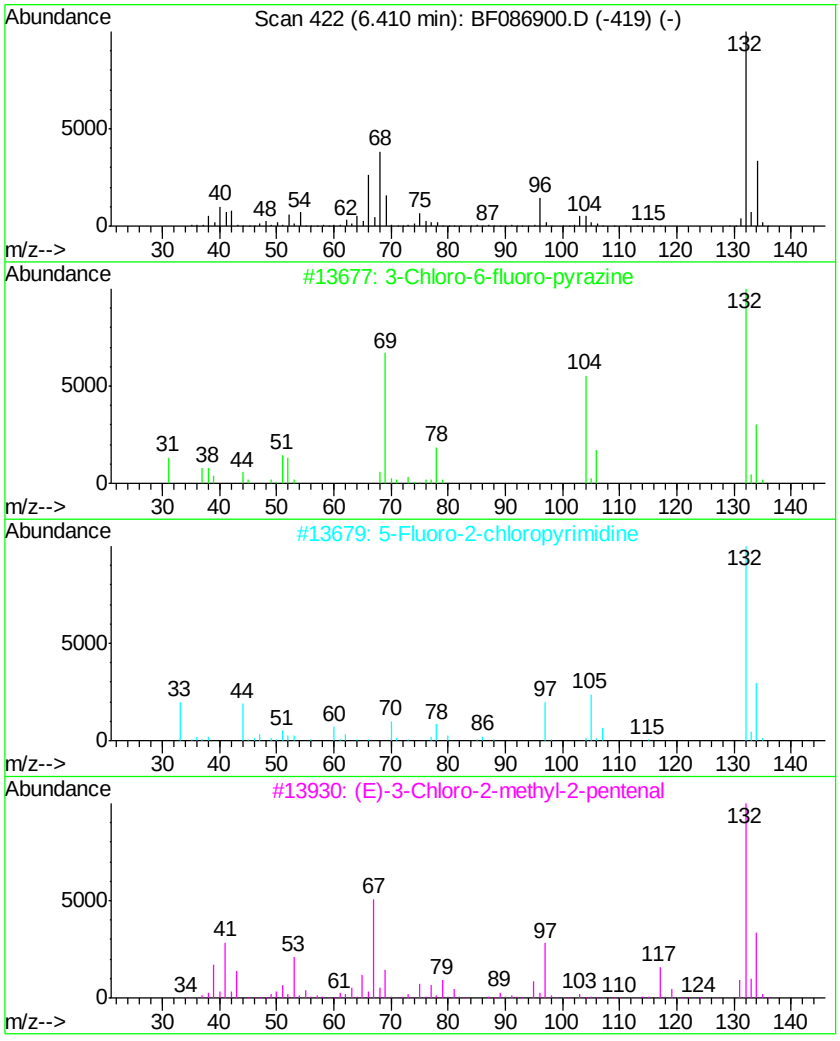
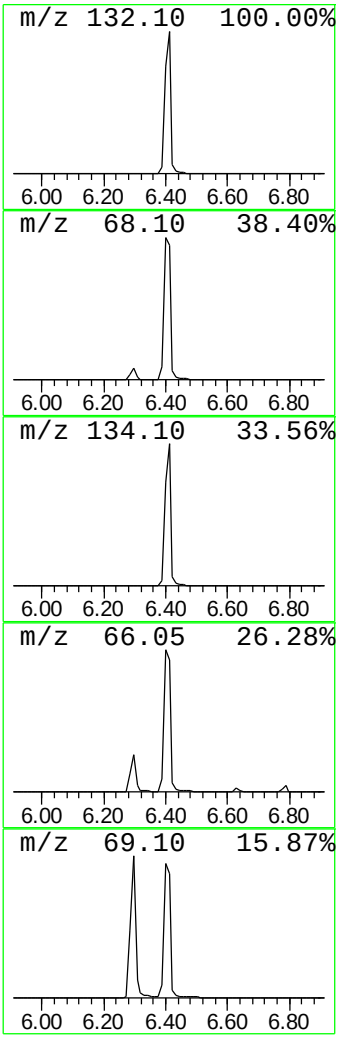
Peak Number 4 unknown6.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	54.72 ng	5453290	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Data File : BF086900.D
Acq On : 11 May 2016 21:05
Operator : UM/SJ
Sample : H2894-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP18-8FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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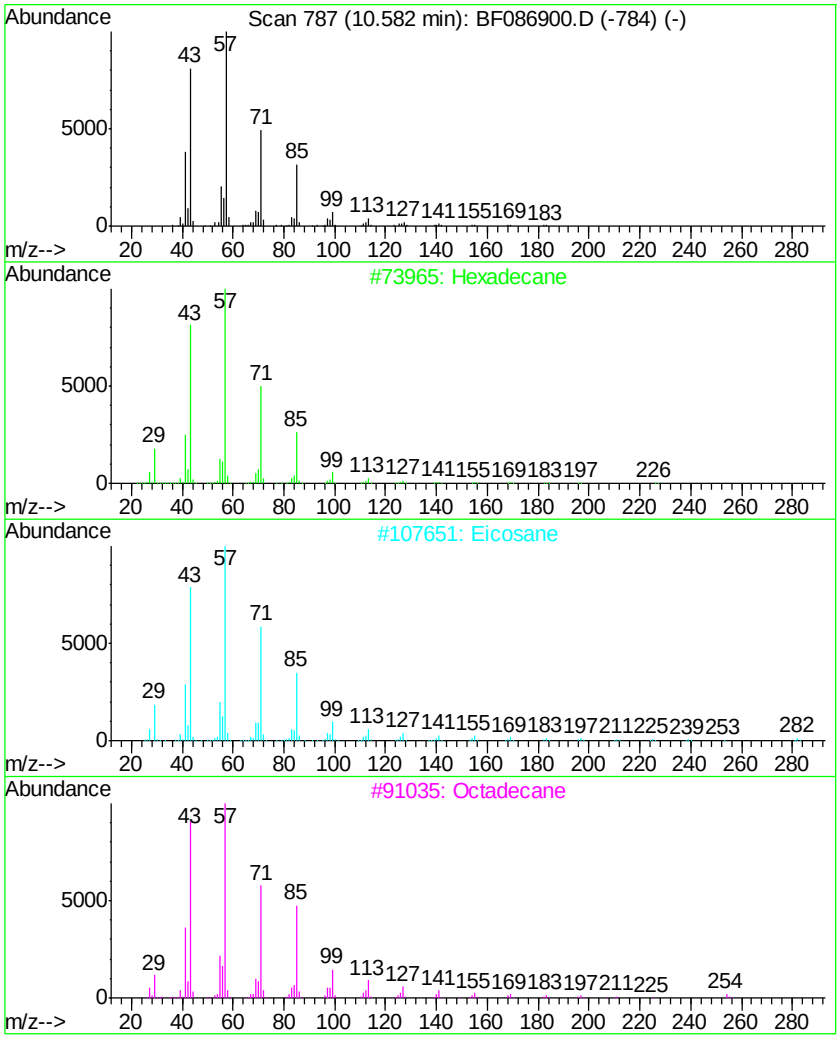
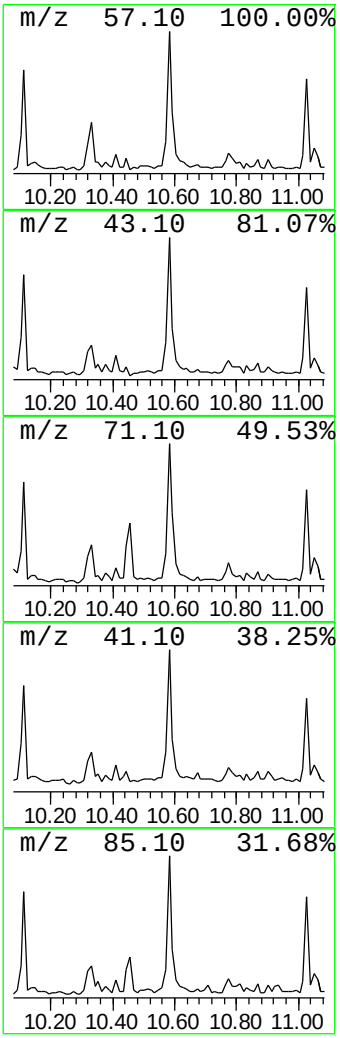
Peak Number 6 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.58	3.24 ng	431347	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	80





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Sample : H2894-01
Misc :
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Instrument : BNA_F
ClientSampleId : TP18-8FT

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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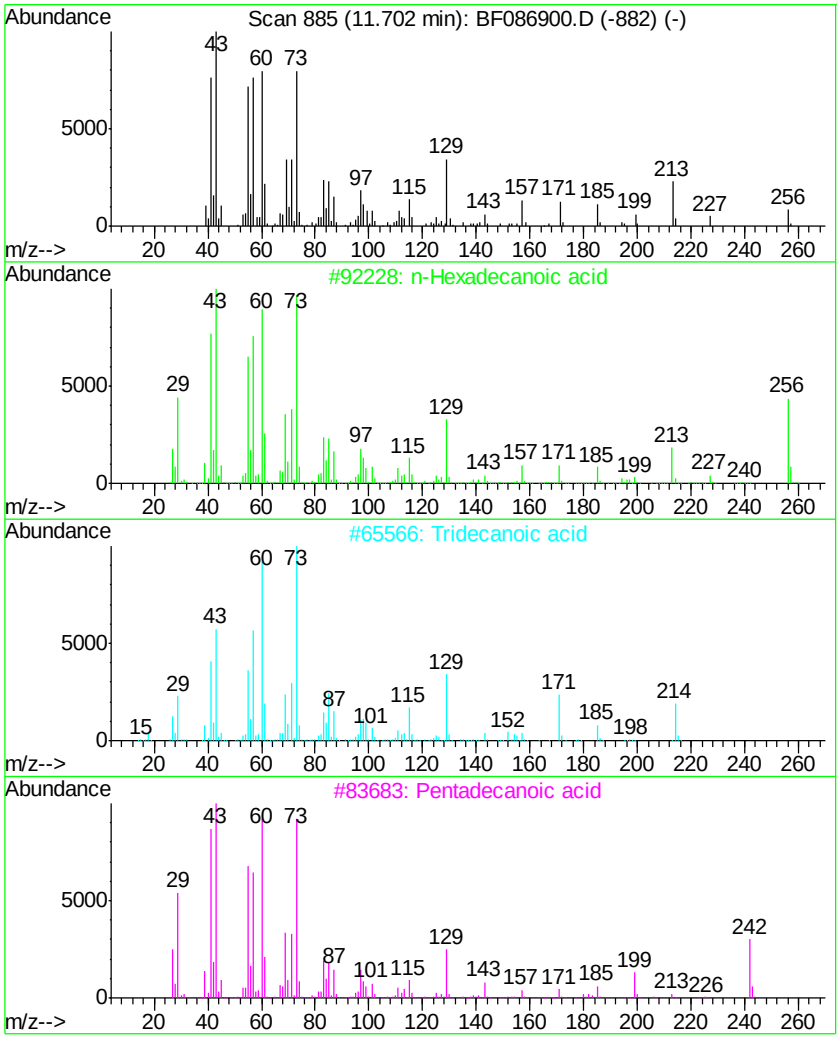
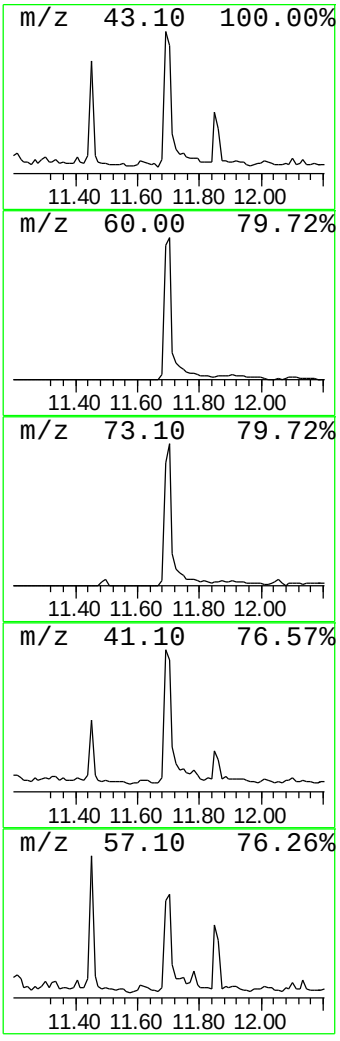
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	4.65 ng	618616	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Tridecanoic acid	214	C13H26O2	000638-53-9	74
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051116\
Data File : BF086900.D
Acq On : 11 May 2016 21:05
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Sample : H2894-01
Misc :
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Instrument : BNA_F
ClientSampleId : TP18-8FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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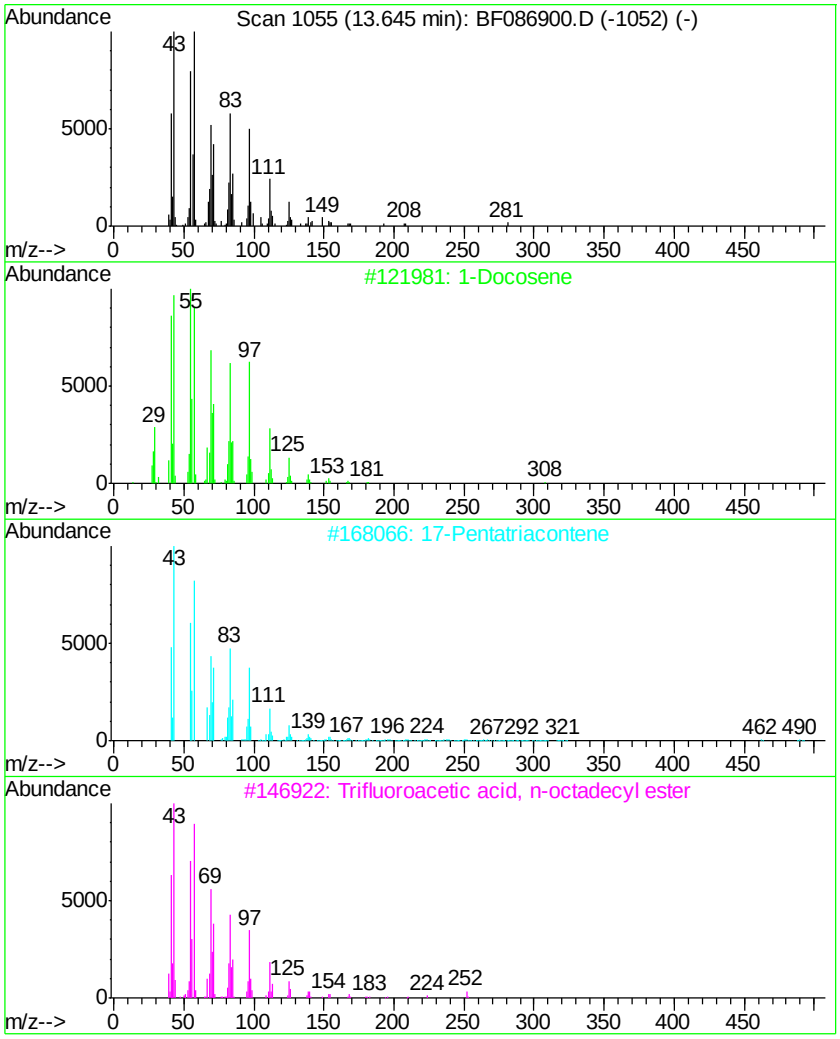
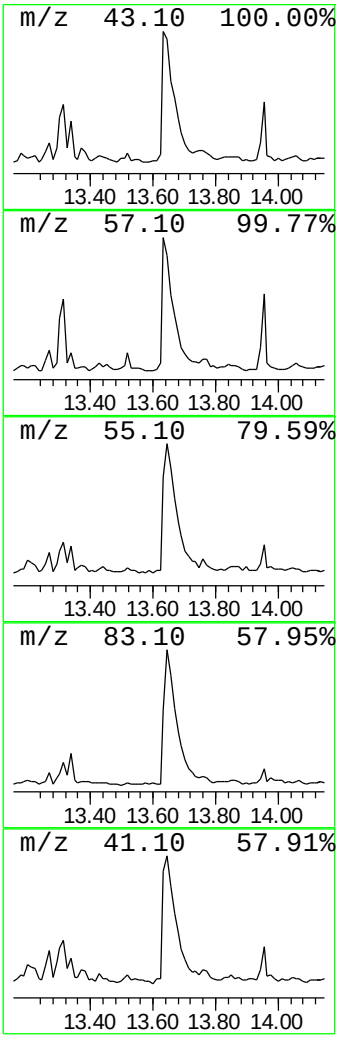
Peak Number 8 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	4.53 ng	573426	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90





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Sample : H2894-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP18-8FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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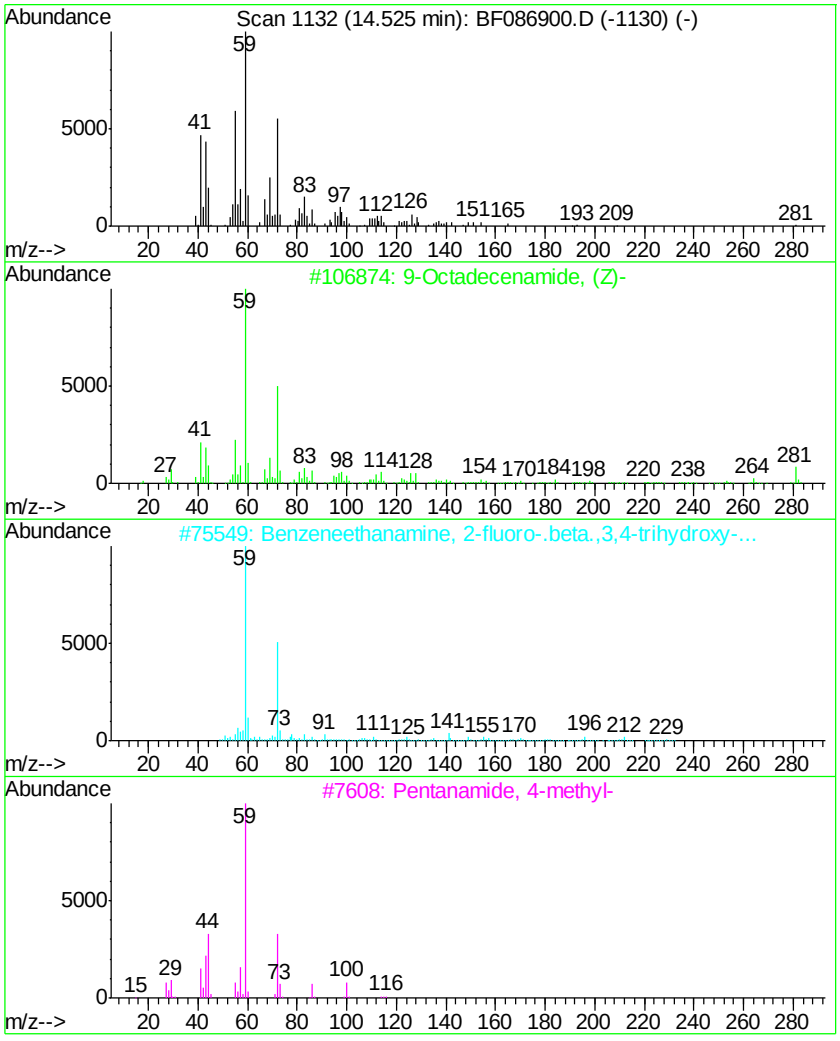
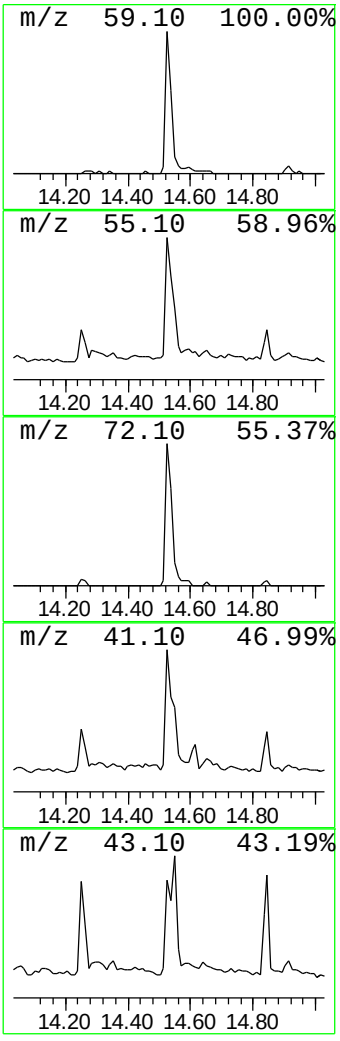
Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	2.73 ng	266188	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
4	Hexadecanamide	255	C16H33NO	000629-54-9	59
5	2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	38





Tentatively Identified Compound (LSC) summary

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Acq On : 11 May 2016 21:05
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Sample : H2894-01
Misc :
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Instrument : BNA_F
ClientSampleId : TP18-8FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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...	4.79	7.7	ng	769609	1	6.63	1993060	20.0
unknown6.41	6.41	54.7	ng	5453290	1	6.63	1993060	20.0
Hexadecane	10.58	3.2	ng	431347	4	11.14	2661410	20.0
n-Hexadecanoic acid	11.70	4.7	ng	618616	4	11.14	2661410	20.0
1-Docosene	13.65	4.5	ng	573426	5	13.77	2531060	20.0
9-Octadecenamide,...	14.53	2.7	ng	266188	6	15.13	1952120	20.0