LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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	5.121	246	248	255	rVB	215942	306563	5.90%	0.703%
2	5.533	280	284	286	rBV	3430147	4373290	84.23%	10.033%
3	6.562	370	374	376	rBV	3667565	4261969	82.08%	9.778%
4	6.699	383	386	388	rBV	3988012	4017613	77.38%	9.217%
5	6.927	404	406	409	rVB	816681	804207	15.49%	1.845%
6	7.087	417	420	423	rBV	3188951	3186998	61.38%	7.312%
7	7.499	453	456	458	rBV	2836582	2927315	56.38%	6.716%
8	8.219	517	519	521	rBV	1351398	1104174	21.27%	2.533%
9	9.305	611	614	616	rBV	4153658	5192166	100.00%	11.912%
10	9.693	646	648	649	rBV	789642	754964	14.54%	1.732%
11	9.910	665	667	669	rBV	127142	111556	2.15%	0.256%
12	9.979	671	673	675	rVB	1374408	1221332	23.52%	2.802%
13	10.402	707	710	712	rBV	121390	181785	3.50%	0.417%
14	10.631	726	730	733	rBV	61820	105307	2.03%	0.242%
15	10.768	739	742	744	rBV	2982136	2985877	57.51%	6.850%
16	10.882	749	752	759	rVV	198766	253352	4.88%	0.581%
17	11.328	789	791	793	rBV	108279	94546	1.82%	0.217%
18	11.465	801	803	804	rBV	1415953	1293497	24.91%	2.968%
19	11.488	804	805	806	rVV	145996	106942	2.06%	0.245%
20	11.533	806	809	811	rVB	36966	57847	1.11%	0.133%
21	11.991	845	849	851	rBV	215754	260517	5.02%	0.598%
22	12.676	906	909	911	rBV	272155	259488	5.00%	0.595%
23	12.779	915	918	924	rVV	163958	304400	5.86%	0.698%
24	12.905	924	929	931	rVV	208577	273346	5.26%	0.627%
25	12.951	931	933	935	rVB2	46387	56735	1.09%	0.130%
26	13.054	939	942	944	rVB	4462149	4272284	82.28%	9.801%
27	13.945	1018	1020	1025	rBV	191013	234071	4.51%	0.537%
28	14.105	1030	1034	1035	rBV	1308655	1474842	28.41%	3.384%
29	14.128	1035	1036	1038	rVB	107743	81753	1.57%	0.188%
30	14.494	1060	1068	1069	rBV	67265	219157	4.22%	0.503%
31	14.574	1073	1075	1087	rVB4	78966	263682	5.08%	0.605%
32	14.734	1087	1089	1091	rBV	955130	938532	18.08%	2.153%
33	14.791	1091	1094	1098	rVB	32844	95885	1.85%	0.220%
34	14.951	1106	1108	1117	rVB2	53221	110755	2.13%	0.254%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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

35	15.134	1122	1124	1129	rVB	69422	139517	2.69%	0.320%
36	15.442	1148	1151	1154	rVB	40235	56760	1.09%	0.130%
37	15.500	1154	1156	1159	rBV	55429	74155	1.43%	0.170%
38	15.568	1159	1162	1168	rVB	725908	932669	17.96%	2.140%
39	16.528	1243	1246	1250	rBV2	22880	53587	1.03%	0.123%
40	17.008	1286	1288	1294	rVB2	23588	58234	1.12%	0.134%
41	17.614	1337	1341	1345	rBV3	36084	86989	1.68%	0.200%

Sum of corrected areas: 43588658

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
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Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
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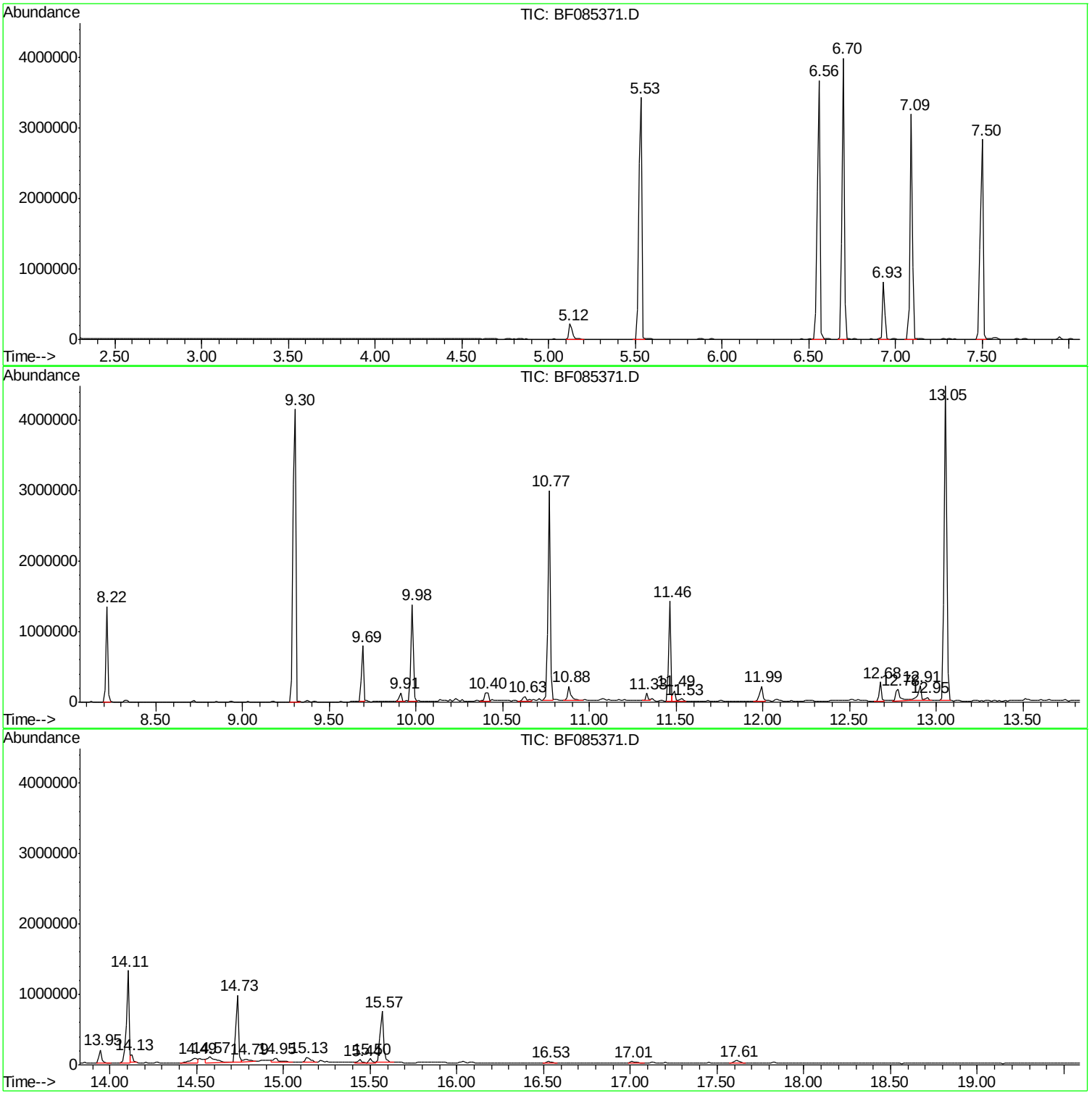
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-18-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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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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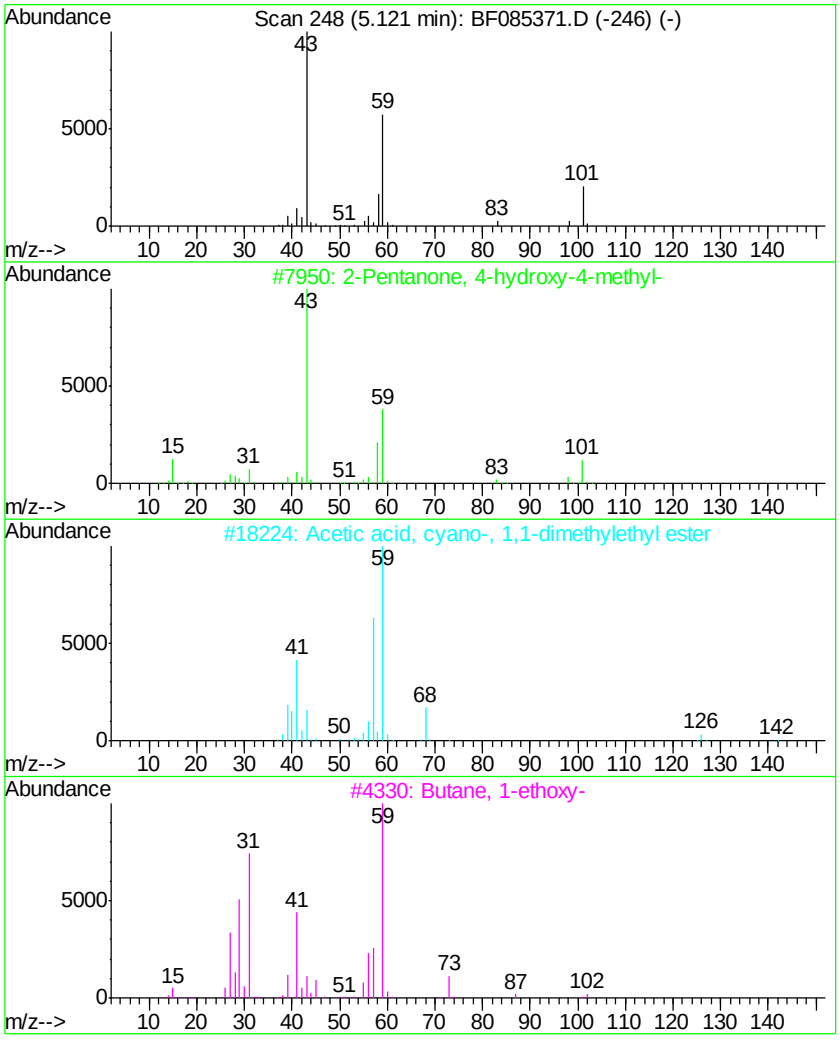
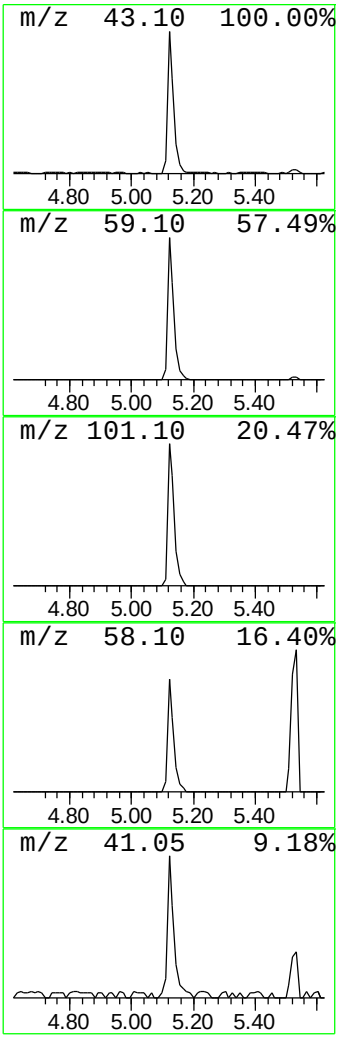
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	7.62 ng	306563	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : H1731-02
Misc :
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Instrument : BNA_F
ClientSampleId : SB-18-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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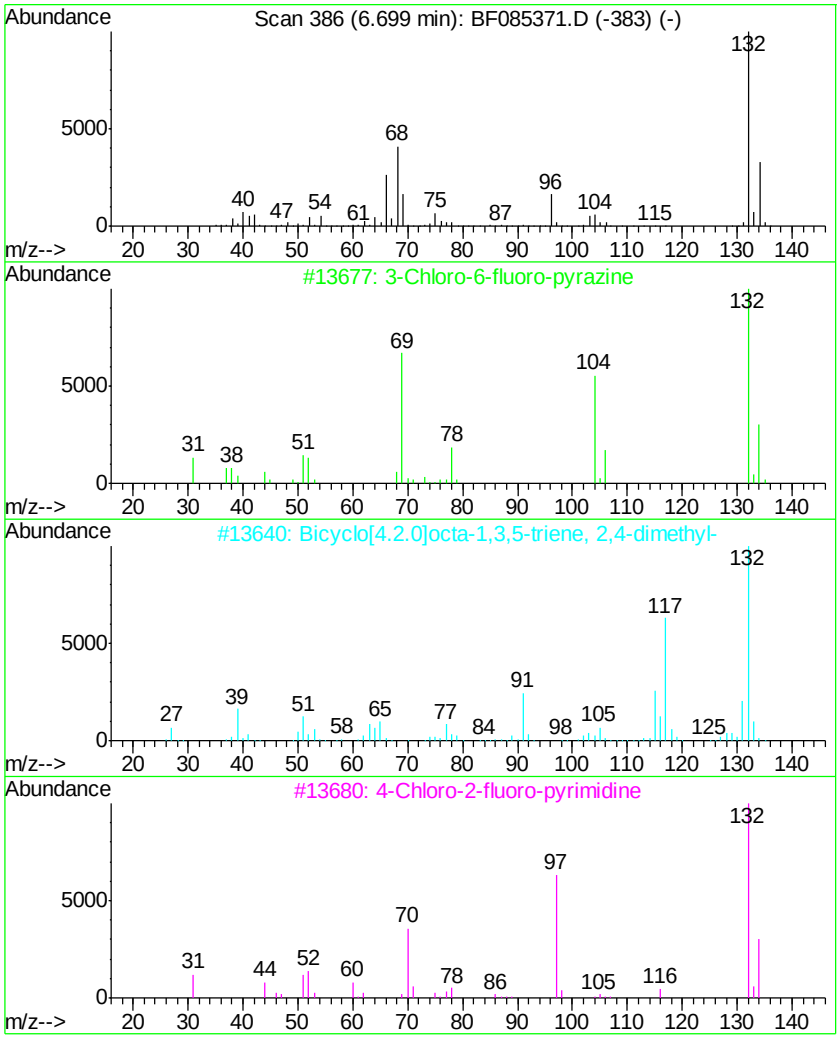
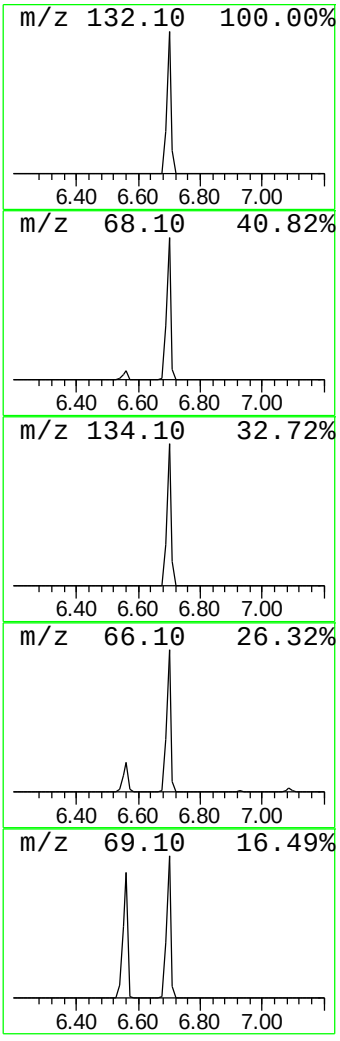
Peak Number 2 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	99.91 ng	4017610	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
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Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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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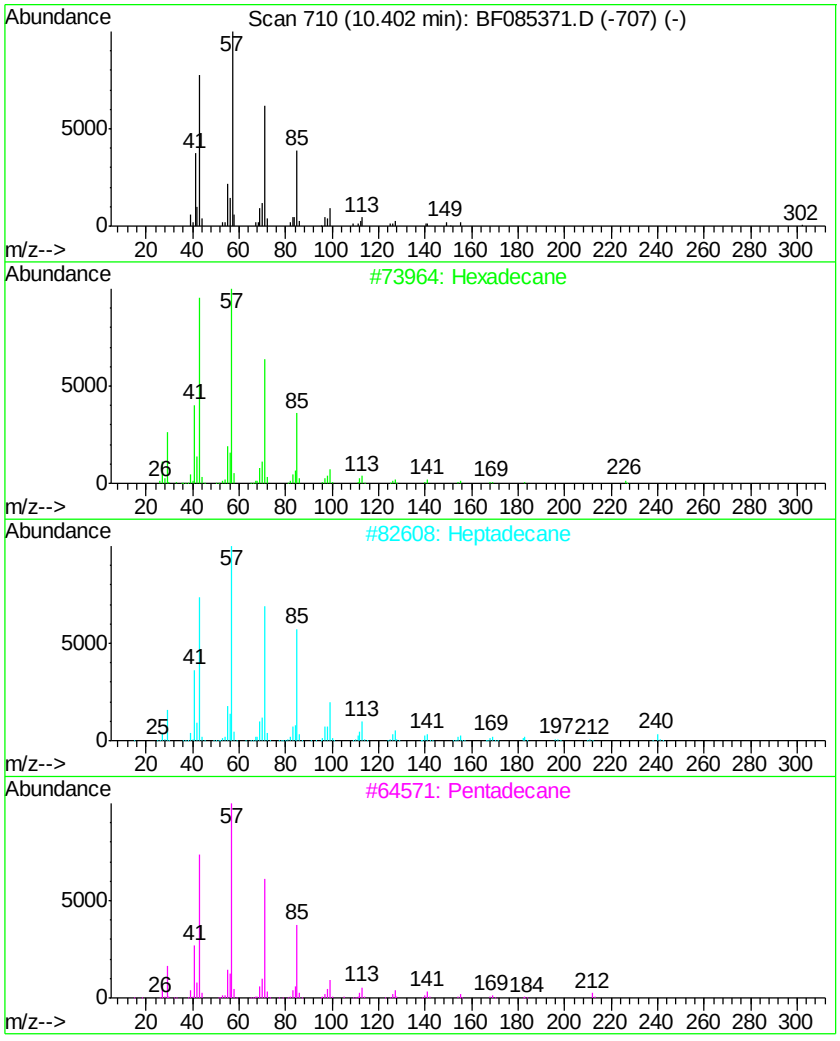
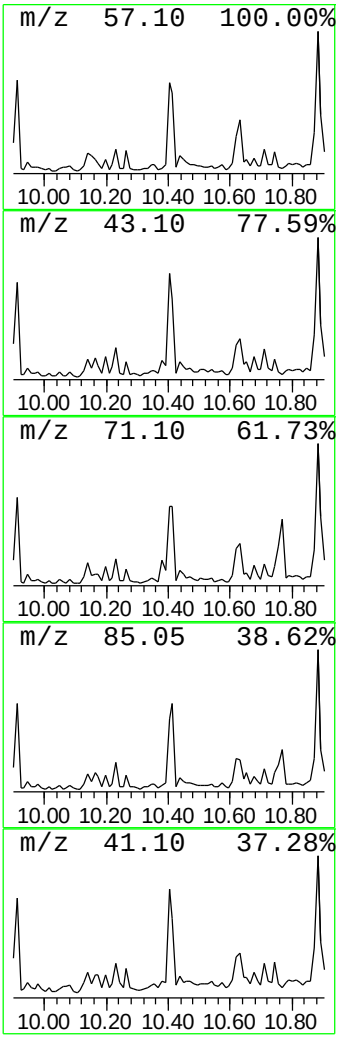
Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.98 ng	181785	Acenaphthene-d10	9.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Heptadecane	240	C17H36	000629-78-7	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	86
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
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Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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
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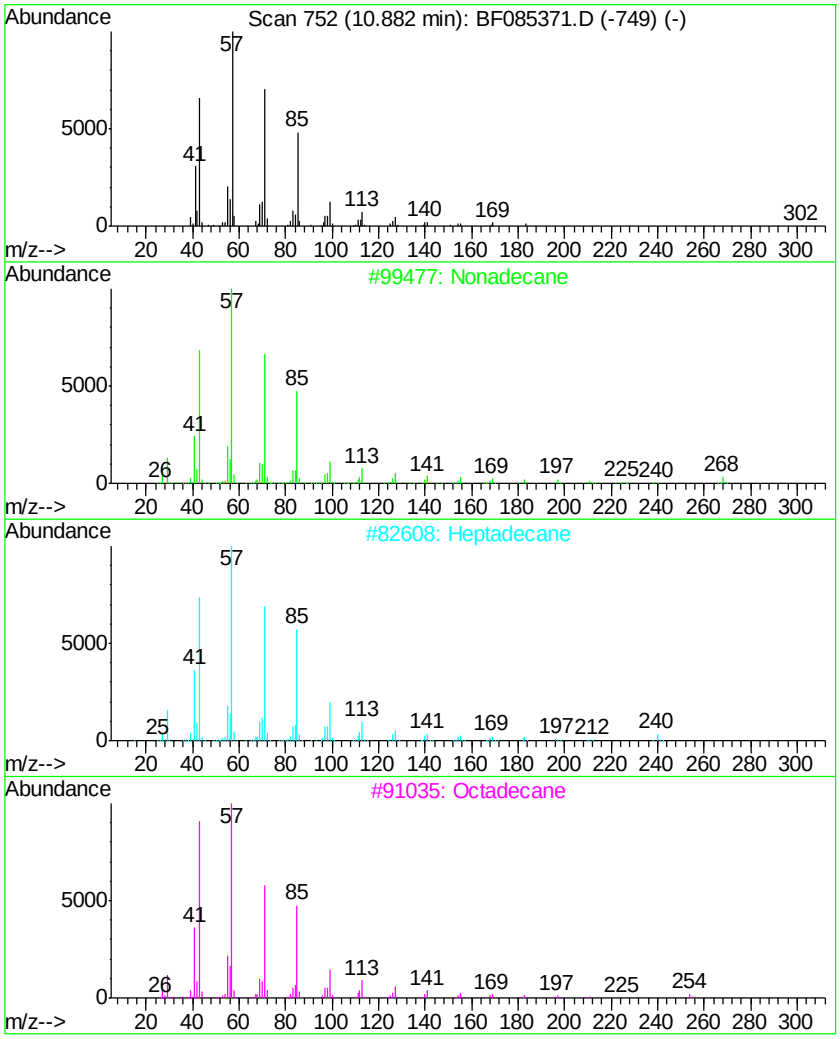
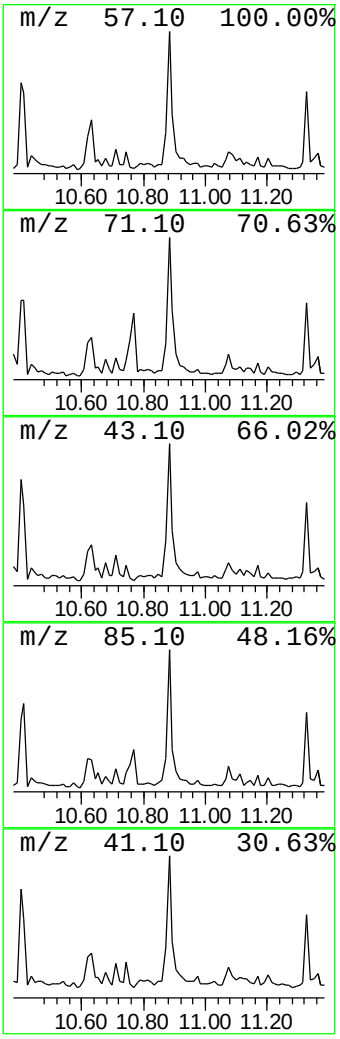
****

Peak Number 5 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	3.92 ng	253352	Phenanthrene-d10	11.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Tetracosane	338	C24H50	000646-31-1	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-COMP

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

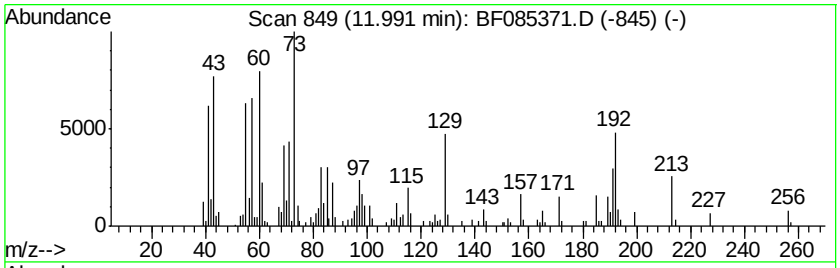
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

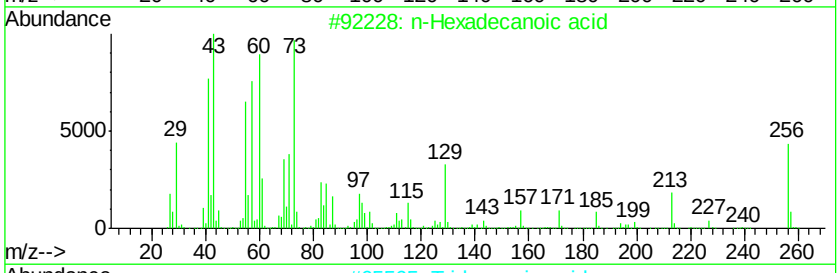
****

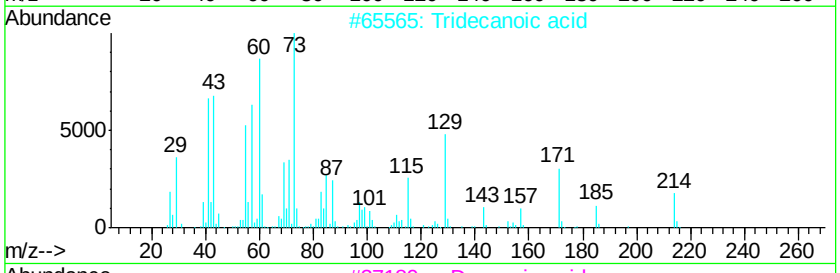
Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

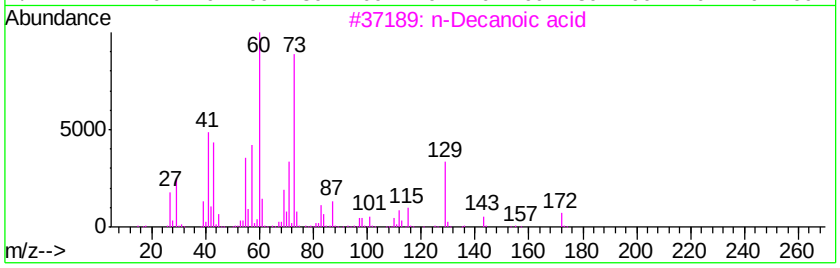
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	4.03 ng	260517	Phenanthrene-d10	11.46

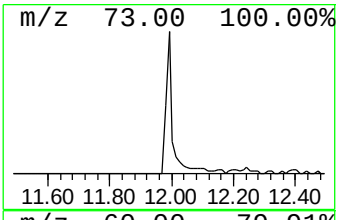
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	30

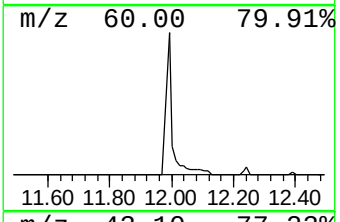


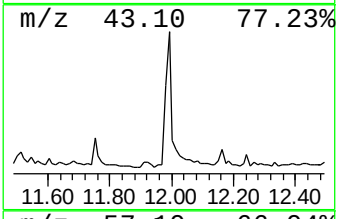


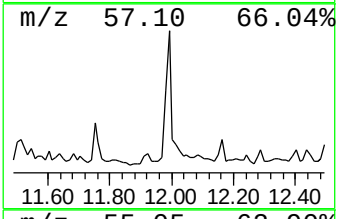


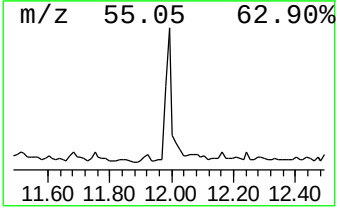












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Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-COMP

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

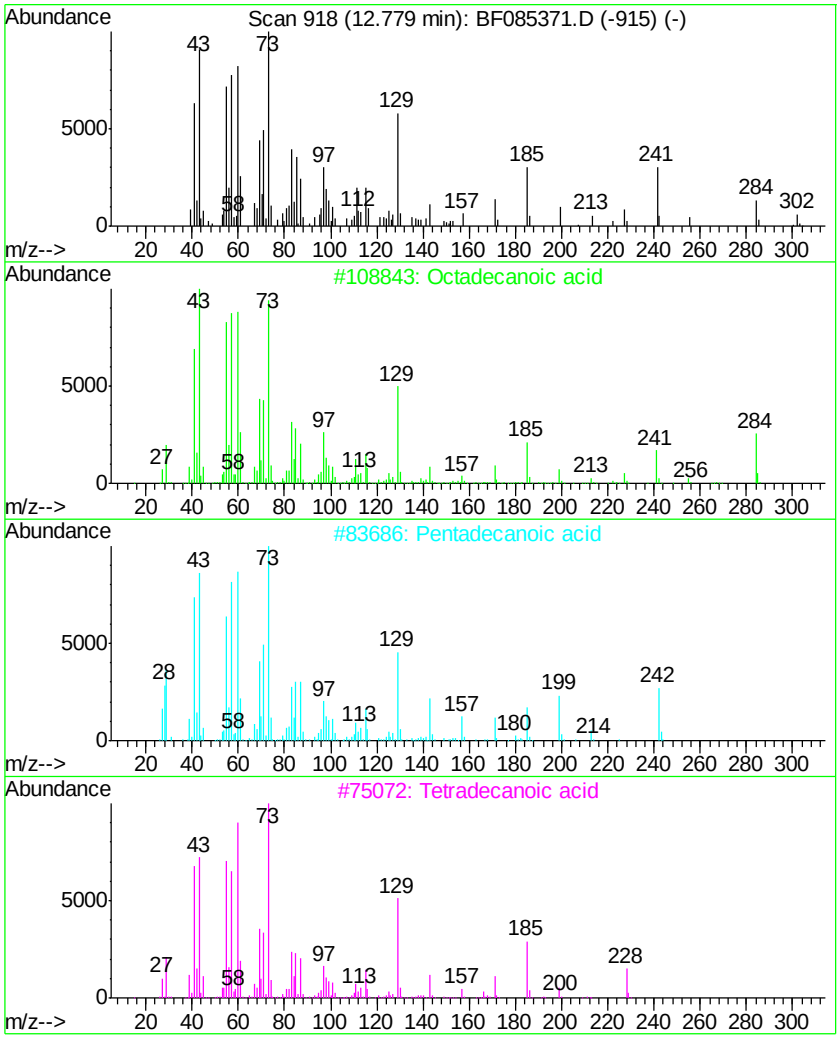
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

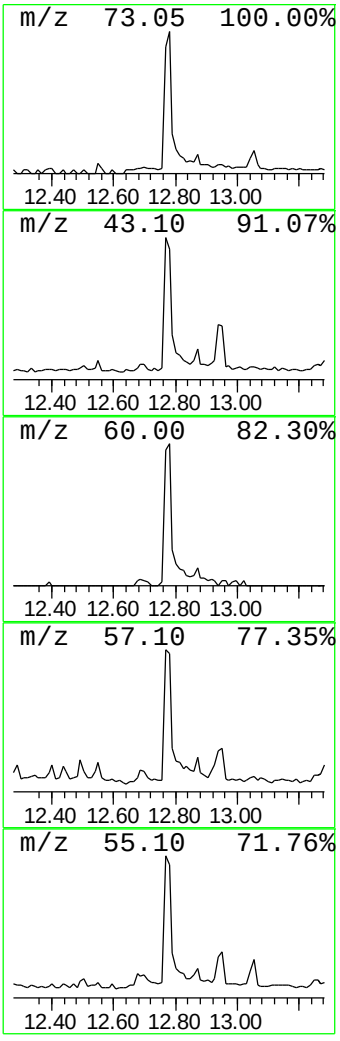
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	4.71 ng	304400	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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	Tridecanoic acid	214	C13H26O2	000638-53-9	50





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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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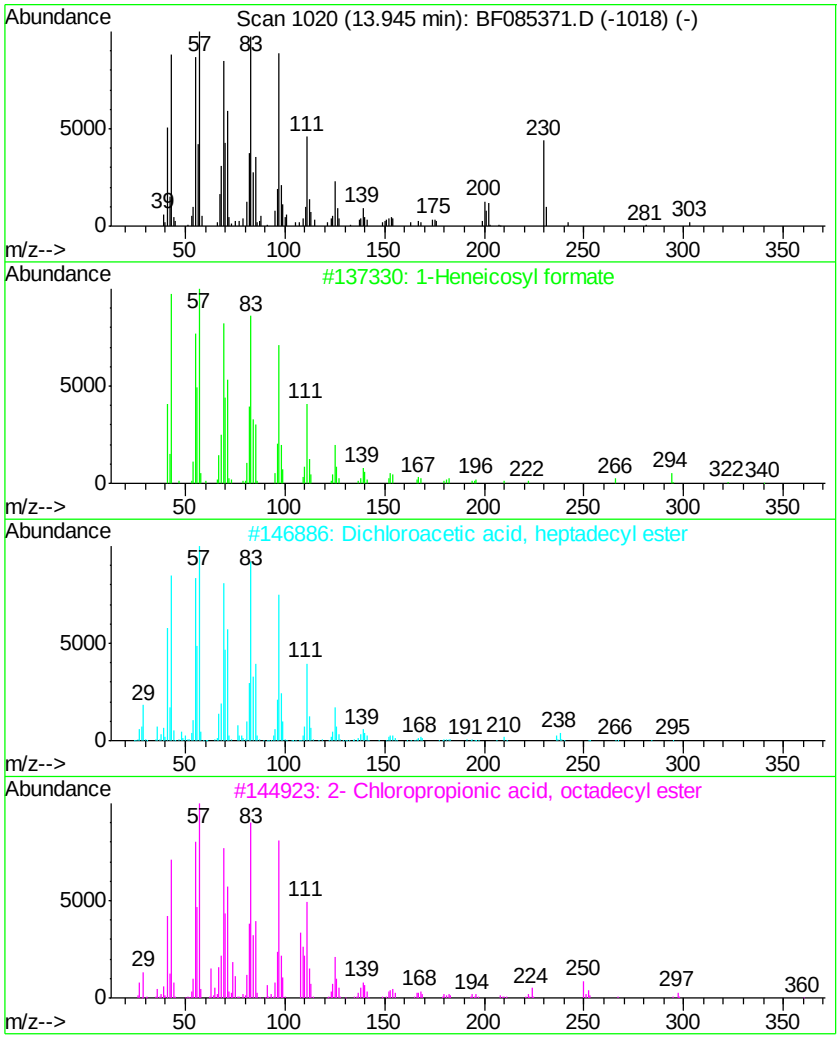
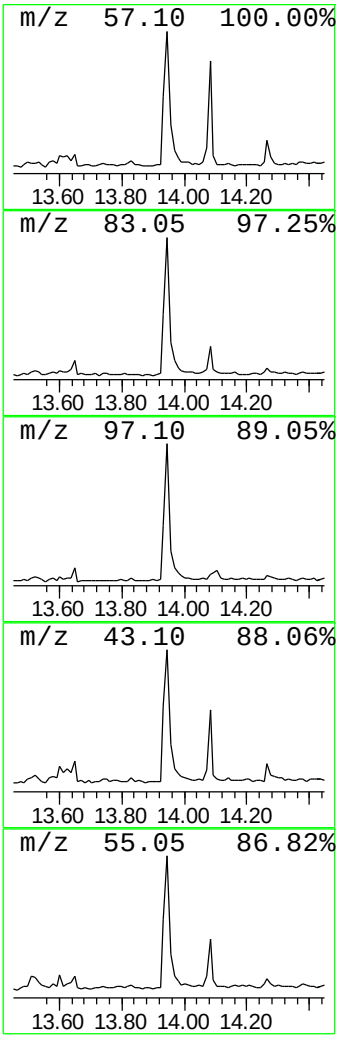
Peak Number 8 1-Heneicosyl formate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.17 ng	234071	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	93





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
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Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-COMP

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TIC Integration Parameters: LSCINT.P

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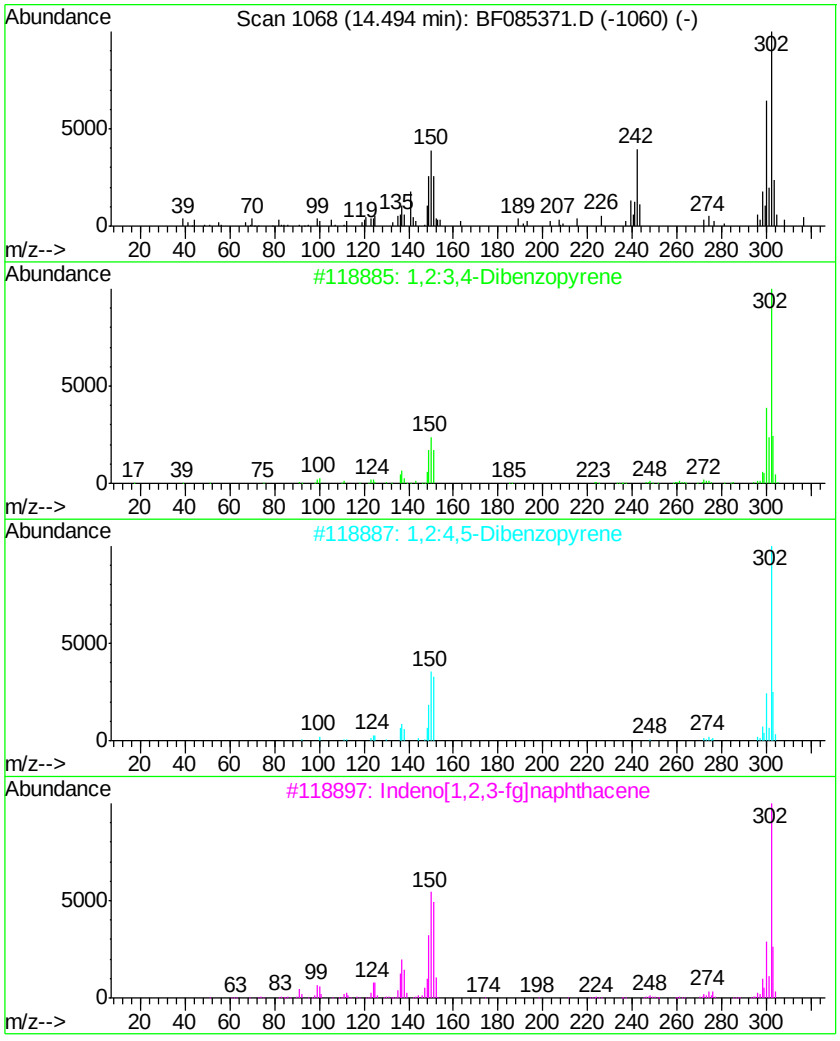
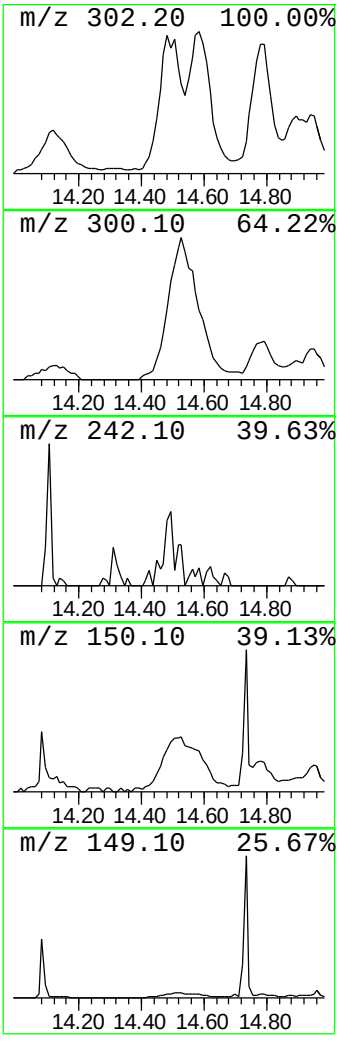
Peak Number 9 1,2:3,4-Dibenzopyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	2.97 ng	219157	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2:3,4-Dibenzopyrene	302	C24H14	000191-30-0	93
2	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	55
3	Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	46
4	3,4:9,10-Dibenzopyrene	302	C24H14	000189-55-9	46
5	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	46





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Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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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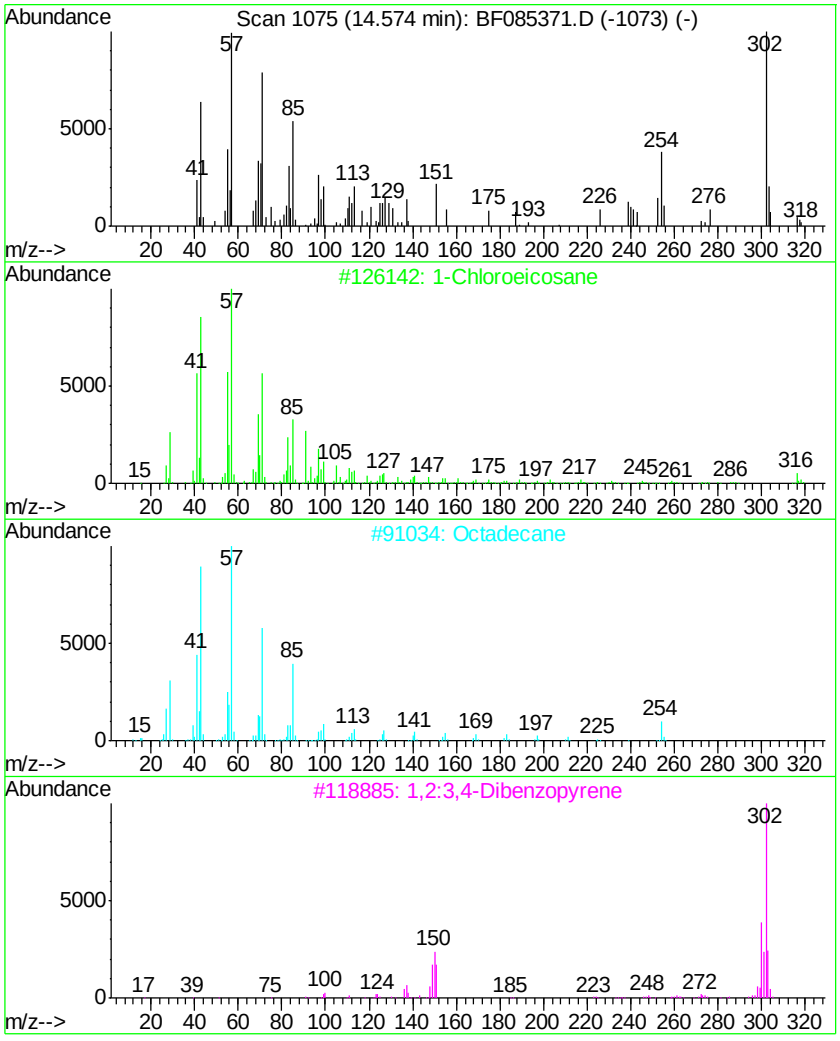
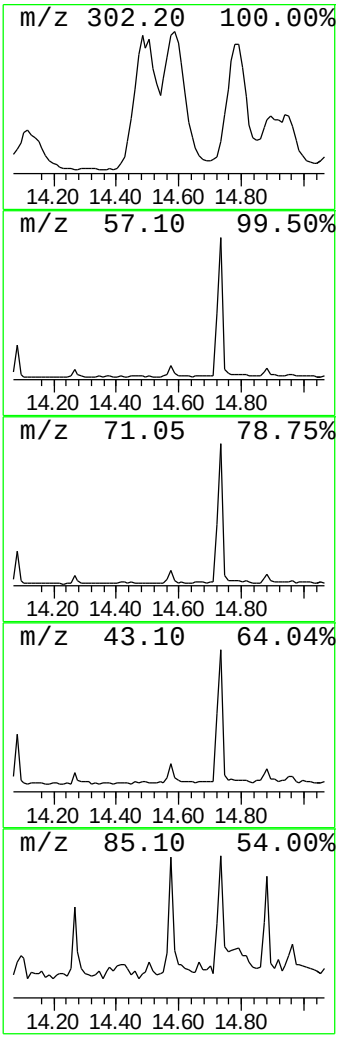
Peak Number 10 1-Chloroeicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.58 ng	263682	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	66
2	Octadecane	254	C18H38	000593-45-3	50
3	1,2:3,4-Dibenzopyrene	302	C24H14	000191-30-0	46
4	Hexadecane	226	C16H34	000544-76-3	46
5	Heptadecane	240	C17H36	000629-78-7	45





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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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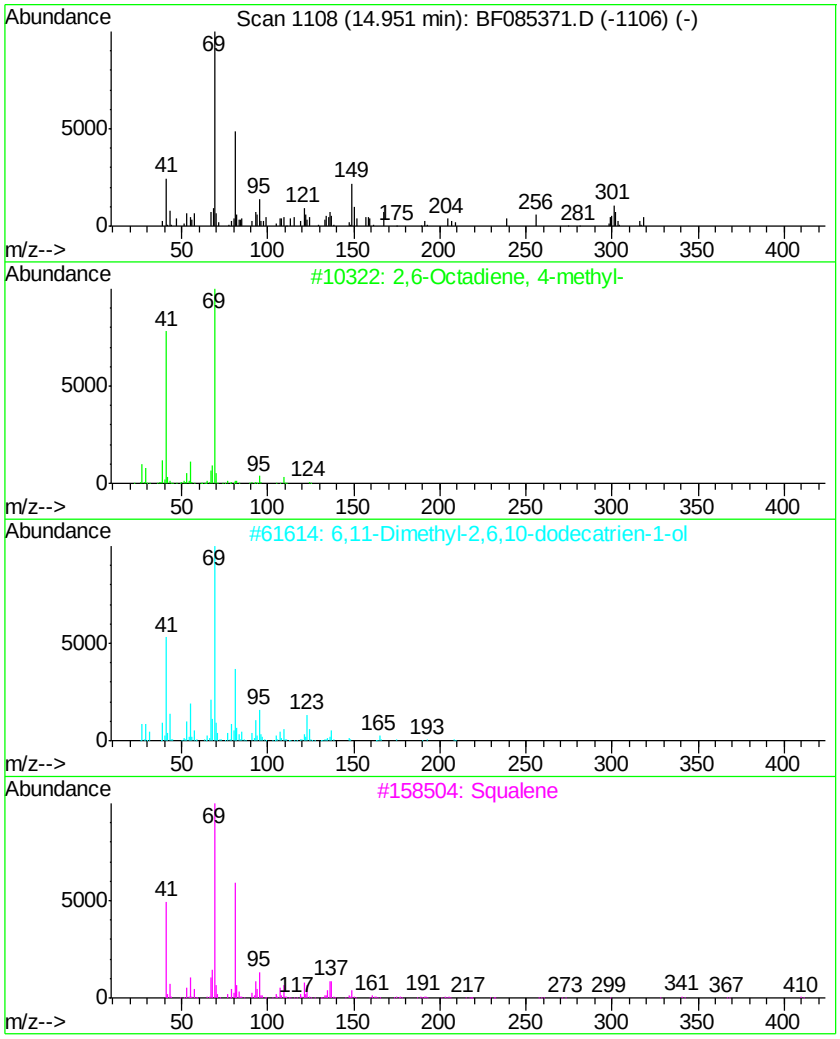
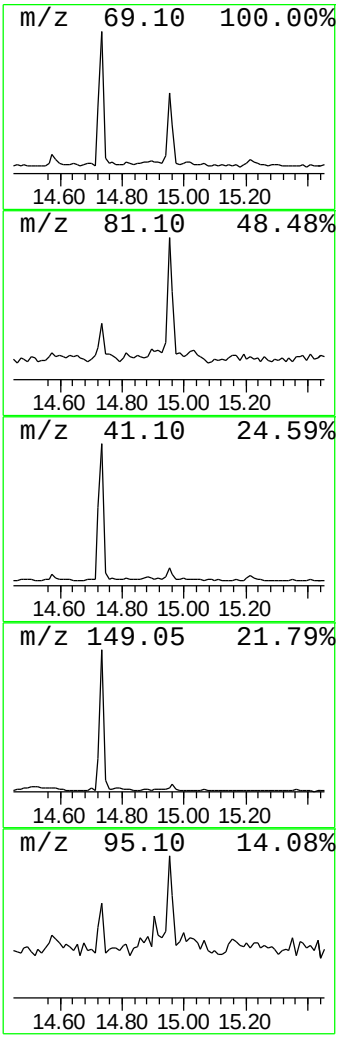
Peak Number 11 unknown14.95 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.38 ng	110755	Perylene-d12	15.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	46
2	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	43
3	Squalene	410	C30H50	007683-64-9	40
4	2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	38
5	Trifluoroacetyl-lavandulol	250	C12H17F3O2	028673-24-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
Data File : BF085371.D
Acq On : 11 Mar 2016 14:44
Operator : UM/SJ
Sample : H1731-02
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-18-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...	5.12	7.6	ng	306563	1	6.93	804207	20.0
unknown6.70	6.70	99.9	ng	4017610	1	6.93	804207	20.0
Hexadecane	10.40	3.0	ng	181785	3	9.98	1221330	20.0
Nonadecane	10.88	3.9	ng	253352	4	11.46	1293500	20.0
n-Hexadecanoic acid	11.99	4.0	ng	260517	4	11.46	1293500	20.0
Octadecanoic acid	12.78	4.7	ng	304400	4	11.46	1293500	20.0
1-Heneicosyl formate	13.95	3.2	ng	234071	5	14.11	1474840	20.0
1,2:3,4-Dibenzopy...	14.49	3.0	ng	219157	5	14.11	1474840	20.0
1-Chloroeicosane	14.57	3.6	ng	263682	5	14.11	1474840	20.0
unknown14.95	14.95	2.4	ng	110755	6	15.57	932669	20.0