LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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	4.538	194	197	201	rBV	53548	61590	1.47%	0.148%
2	5.167	249	252	258	rBV	844870	1156410	27.53%	2.778%
3	5.567	284	287	290	rBV	3410667	3698760	88.05%	8.884%
4	6.584	373	376	378	rBV	3439810	3728447	88.75%	8.955%
5	6.722	386	388	391	rBV	3071638	4200945	100.00%	10.090%
6	6.962	407	409	411	rBV	964894	957621	22.80%	2.300%
7	7.122	420	423	425	rBV	2464135	3289374	78.30%	7.901%
8	7.522	455	458	460	rBV	2661424	2681868	63.84%	6.441%
9	7.590	462	464	467	rVB	34900	47959	1.14%	0.115%
10	8.242	519	521	524	rBV	1433009	1227052	29.21%	2.947%
11	9.316	612	615	618	rBV	2953833	3793093	90.29%	9.110%
12	9.716	648	650	651	rVB	644978	736833	17.54%	1.770%
13	9.933	666	669	670	rVB	84099	108253	2.58%	0.260%
14	10.002	672	675	677	rVV	1369382	1247179	29.69%	2.996%
15	10.425	711	712	714	rVB	191743	157730	3.75%	0.379%
16	10.642	729	731	735	rBV	53670	102972	2.45%	0.247%
17	10.791	741	744	746	rBV	2347723	2509309	59.73%	6.027%
18	10.905	752	754	758	rBV	139948	222675	5.30%	0.535%
19	11.088	768	770	775	rBV4	27971	78407	1.87%	0.188%
20	11.351	790	793	794	rBV	87069	93195	2.22%	0.224%
21	11.373	794	795	798	rVB	30636	43518	1.04%	0.105%
22	11.488	802	805	808	rBV	1063628	1479904	35.23%	3.555%
23	11.556	808	811	813	rVB	89154	98677	2.35%	0.237%
24	11.705	822	824	829	rBV6	24731	51071	1.22%	0.123%
25	11.979	846	848	849	rBV	39344	47567	1.13%	0.114%
26	12.002	849	850	853	rVV2	328831	486854	11.59%	1.169%
27	12.094	856	858	862	rVB2	83113	130089	3.10%	0.312%
28	12.265	870	873	880	rVB3	35421	116256	2.77%	0.279%
29	12.688	908	910	913	rBV	372956	519108	12.36%	1.247%
30	12.791	917	919	923	rBV	283288	322952	7.69%	0.776%
31	12.916	927	930	933	rVV2	316026	490533	11.68%	1.178%
32	13.065	941	943	946	rVB	2751058	2879949	68.55%	6.917%
33	13.145	946	950	953	rBV3	28995	54232	1.29%	0.130%
34	13.248	956	959	961	rVV	72536	87787	2.09%	0.211%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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	13.351	966	968	972	rVB2	45780	67273	1.60%	0.162%
36	13.637	990	993	998	rBV4	19761	75623	1.80%	0.182%
37	13.865	1010	1013	1015	rBV	36331	63362	1.51%	0.152%
38	13.957	1019	1021	1026	rVB	483160	619669	14.75%	1.488%
39	14.117	1031	1035	1042	rVV2	1065722	1434626	34.15%	3.446%
40	14.597	1074	1077	1078	rBV	48176	74808	1.78%	0.180%
41	14.974	1107	1110	1115	rVB2	53177	99168	2.36%	0.238%
42	15.157	1123	1126	1131	rBV	171019	362899	8.64%	0.872%
43	15.454	1150	1152	1155	rVB	94689	133937	3.19%	0.322%
44	15.522	1155	1158	1161	rVV	114917	169020	4.02%	0.406%
45	15.580	1161	1163	1169	rVB	559856	902396	21.48%	2.167%
46	16.105	1207	1209	1216	rVB6	52369	157372	3.75%	0.378%
47	17.043	1288	1291	1297	rVB2	64458	132786	3.16%	0.319%
48	17.225	1304	1307	1310	rBV	17658	58736	1.40%	0.141%
49	17.477	1326	1329	1337	rVB	51942	129968	3.09%	0.312%
50	17.648	1340	1344	1348	rBV5	25875	92049	2.19%	0.221%
51	18.460	1412	1415	1422	rVB6	17685	55051	1.31%	0.132%
52	18.677	1429	1434	1442	rBV8	22661	97702	2.33%	0.235%

Sum of corrected areas: 41634614

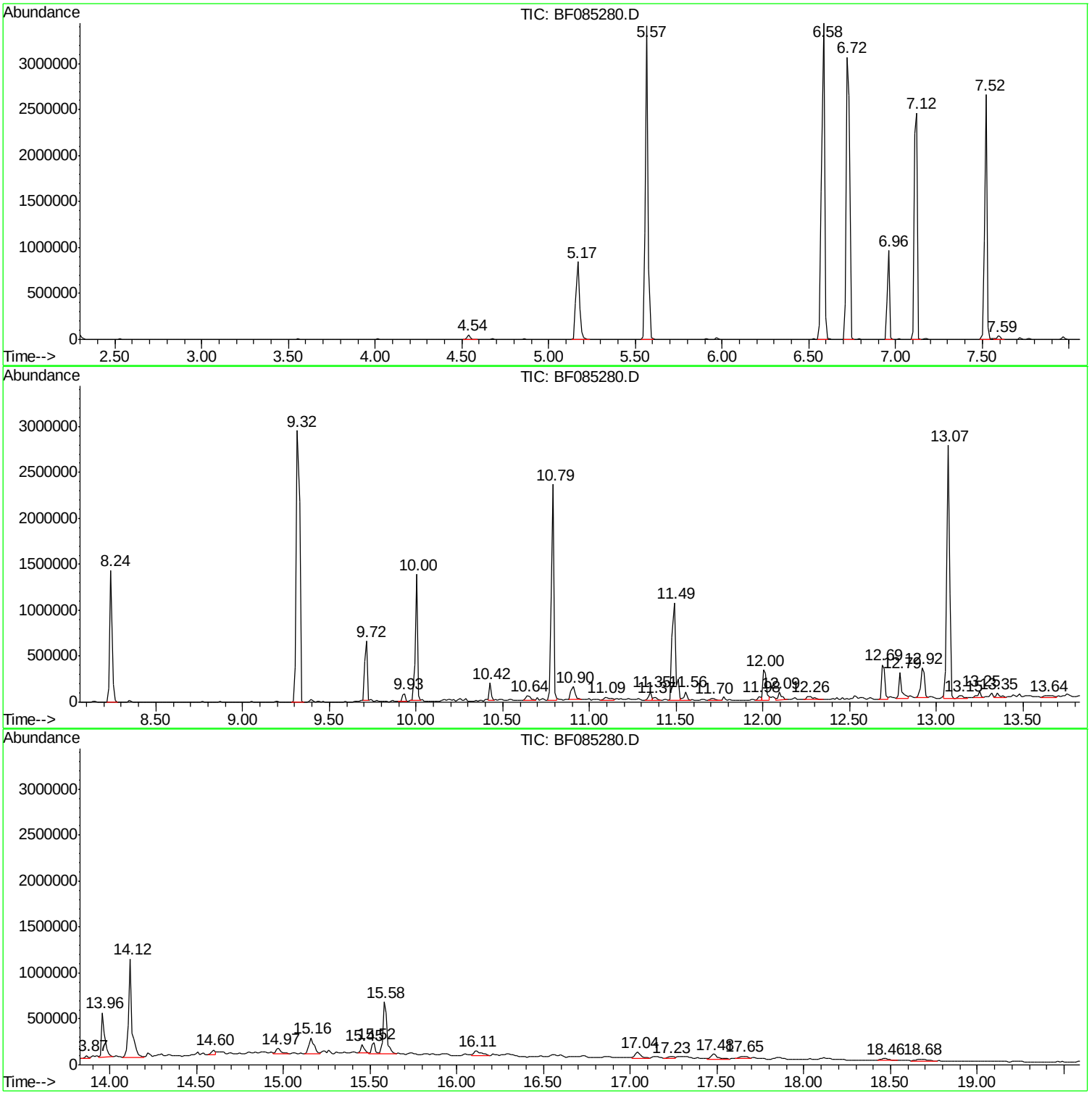
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-39COMP(0.5-2.0)

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\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

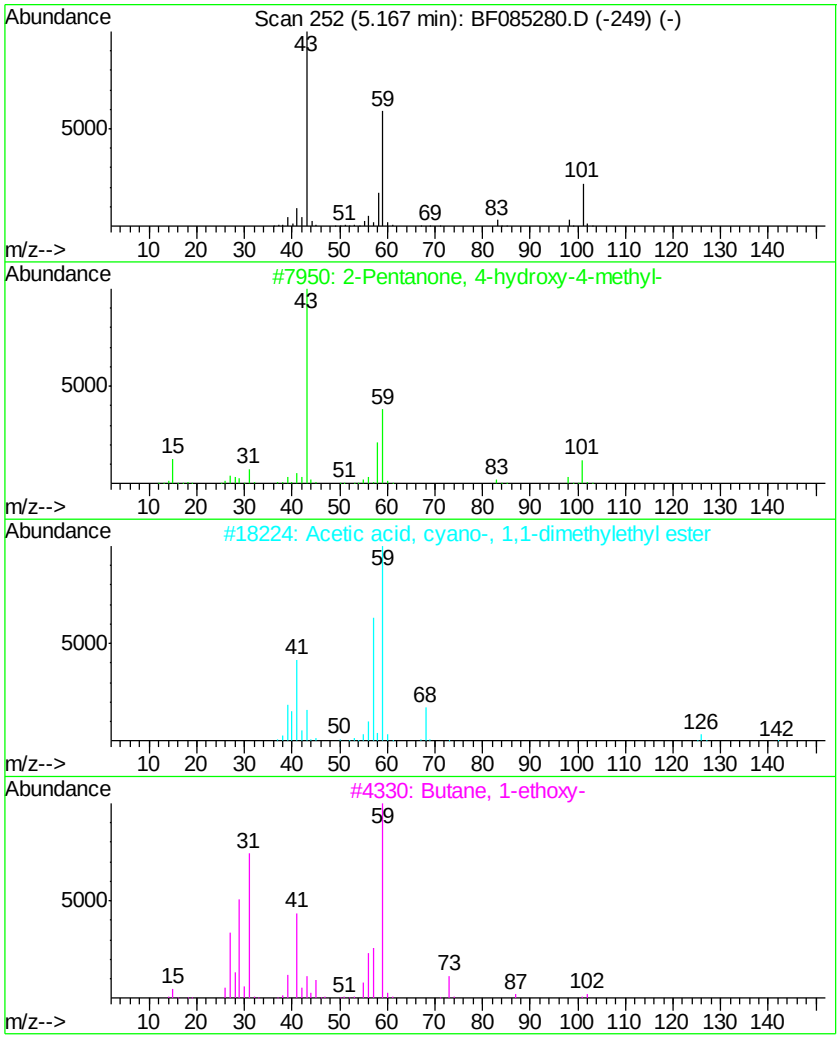
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

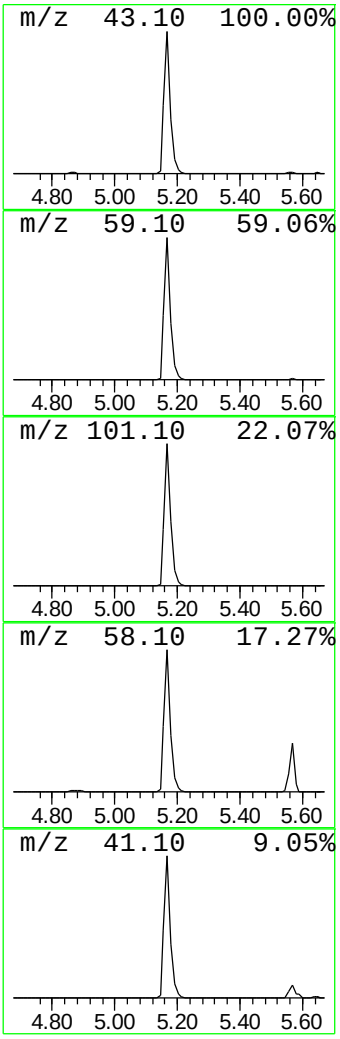
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	24.15 ng	1156410	1,4-Dichlorobenzene-d4	6.96

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-39COMP(0.5-2.0)

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

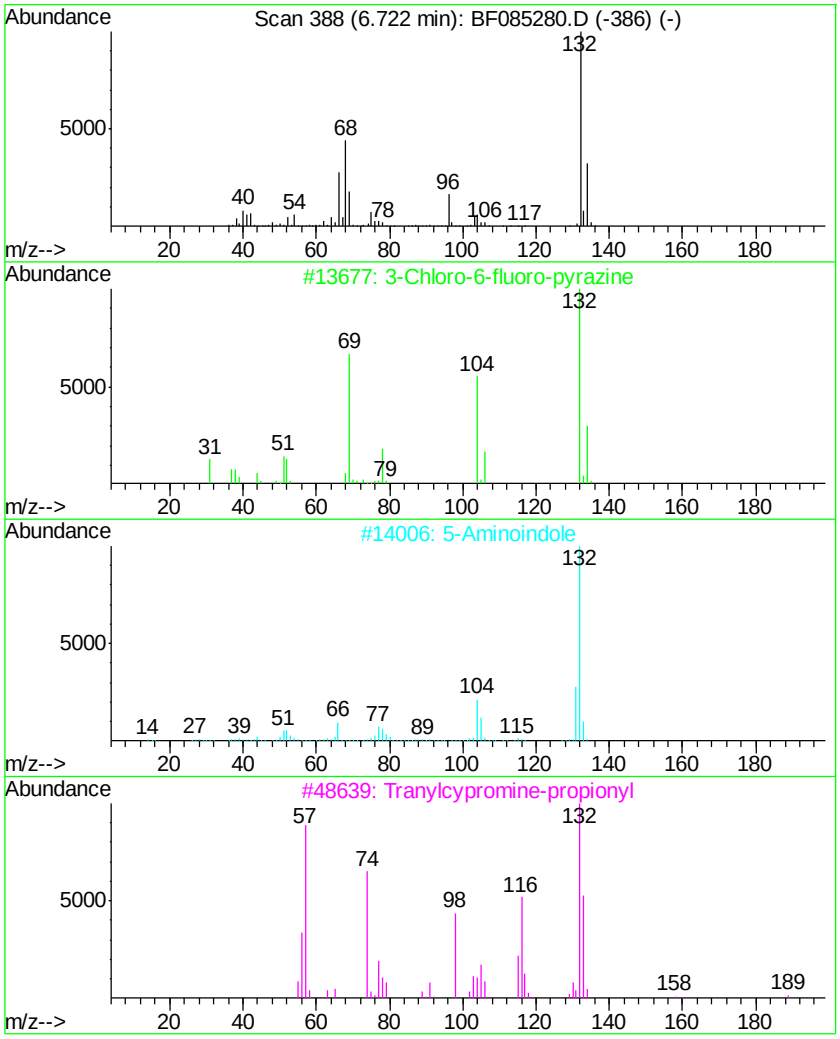
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

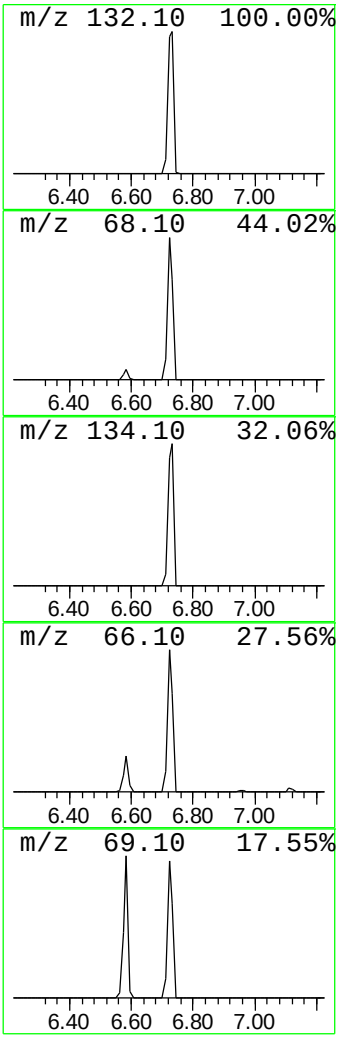
****

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	87.74 ng	4200950	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

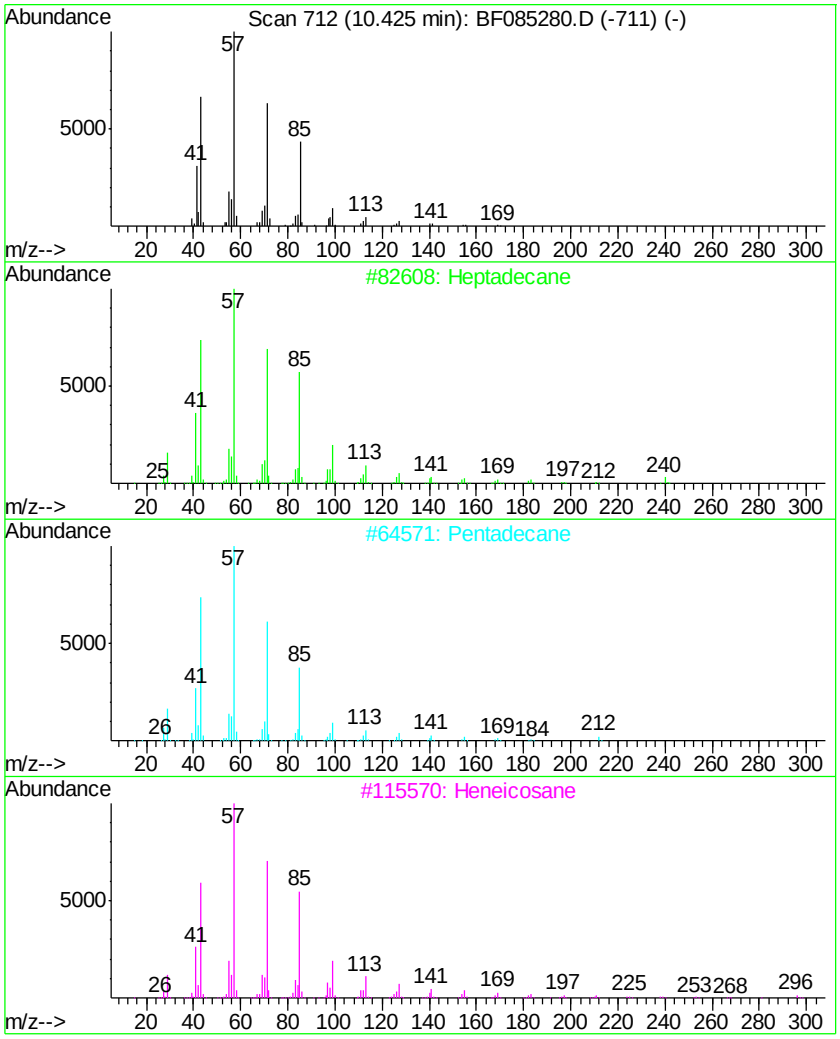
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

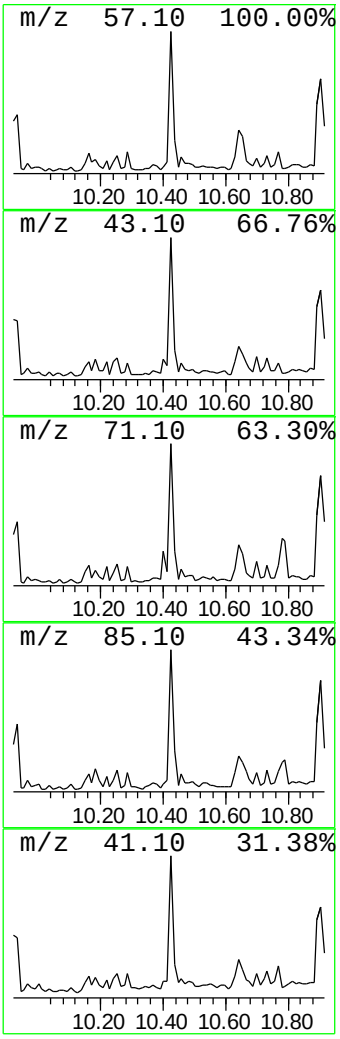
****

Peak Number 4 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.53 ng	157730	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Pentadecane	212	C15H32	000629-62-9	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Eicosane	282	C20H42	000112-95-8	83
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

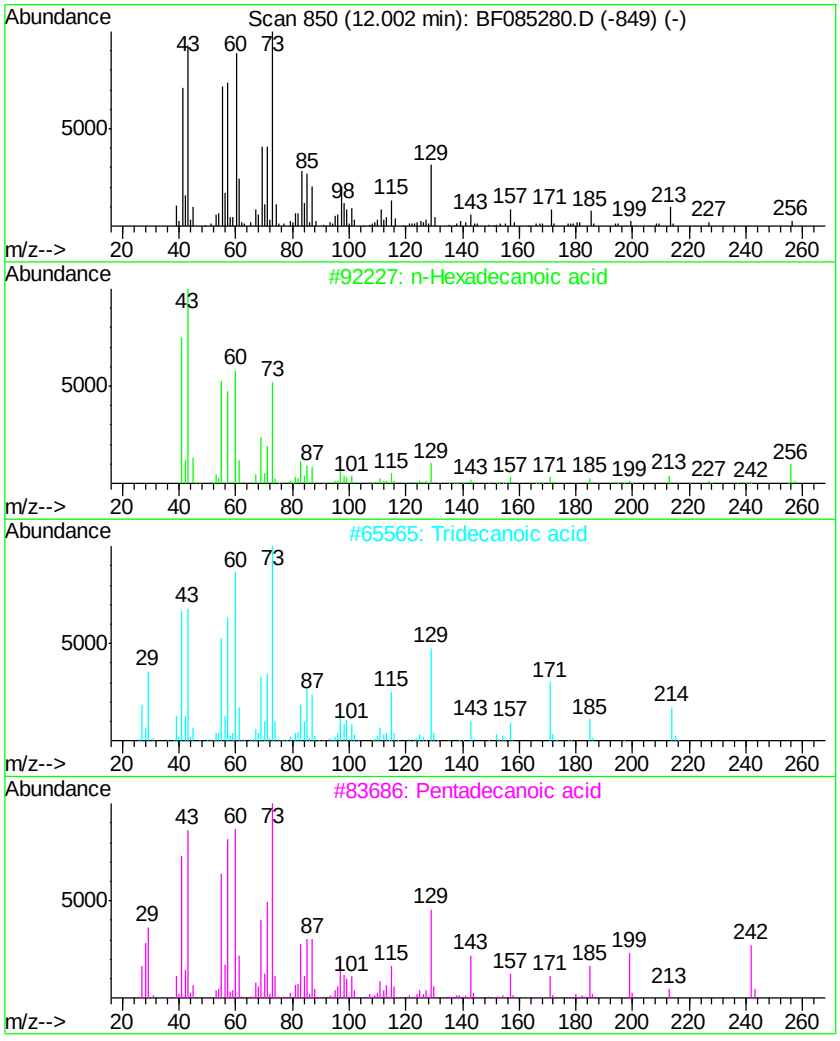
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

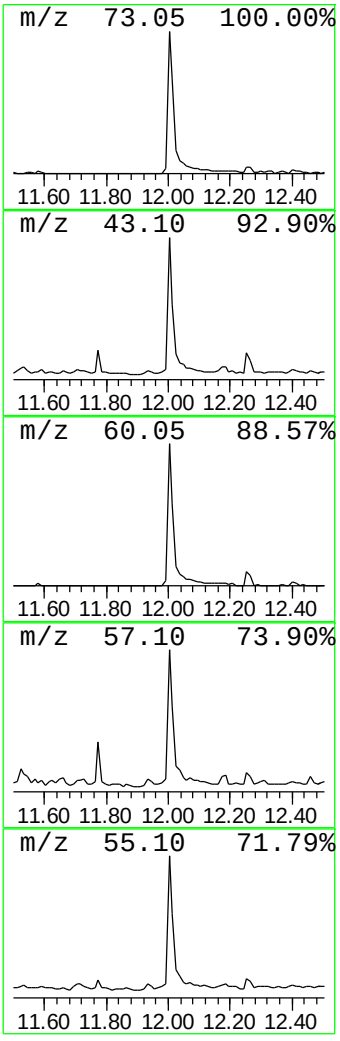
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	6.58 ng	486854	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecane	156	C11H24	001120-21-4	11





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

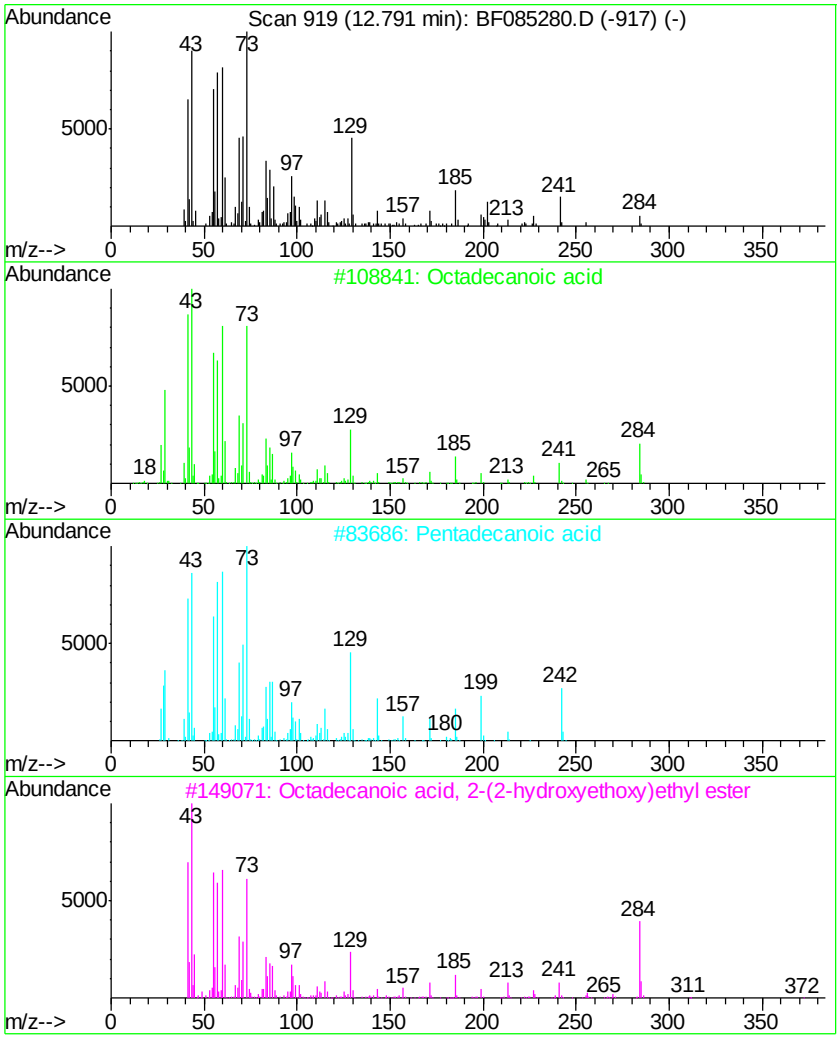
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

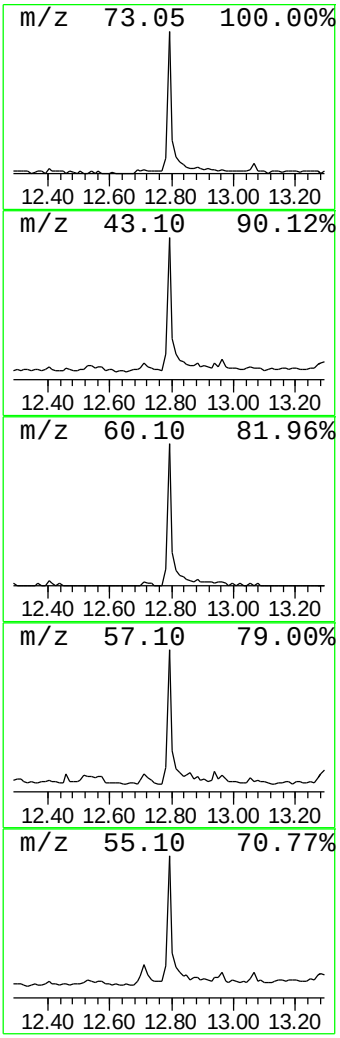
****

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	4.36 ng	322952	Phenanthrene-d10	11.49

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	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

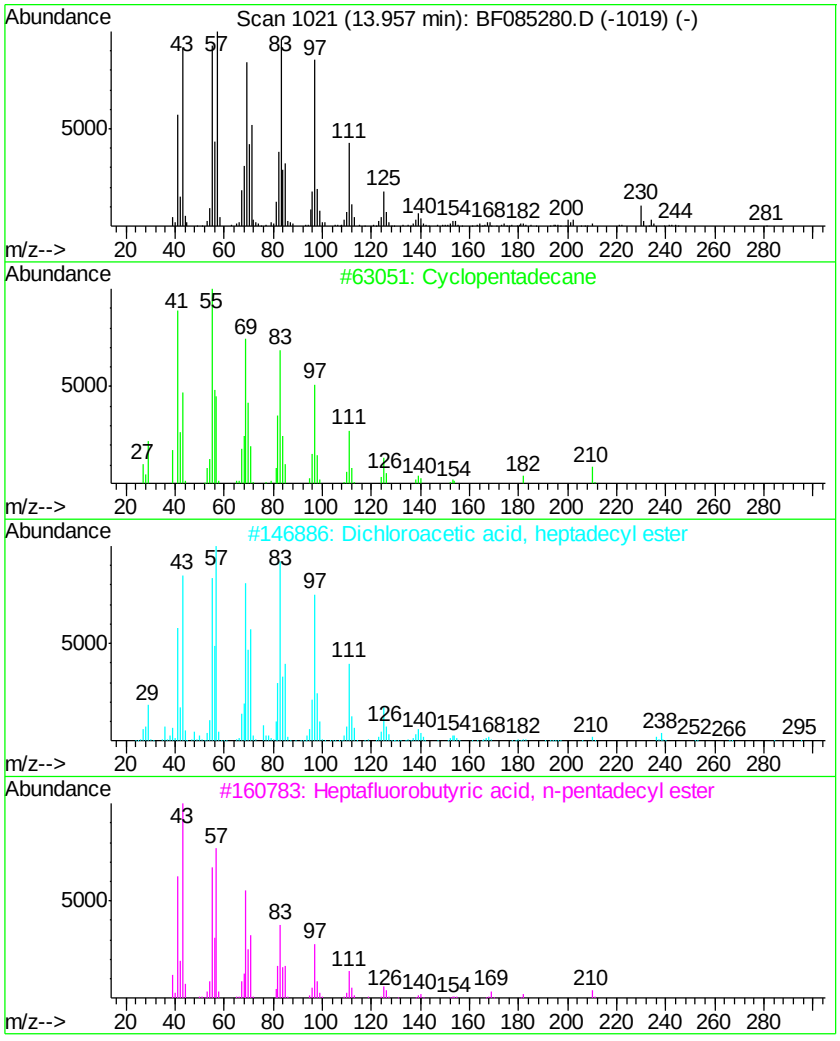
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

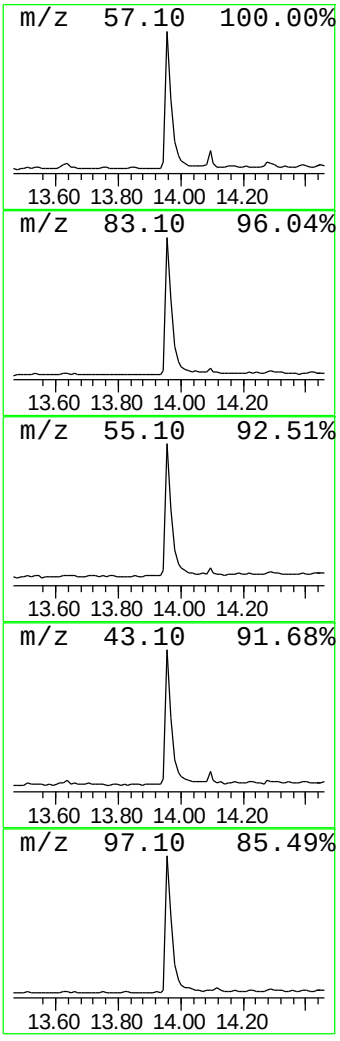
****

Peak Number 8 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	8.64 ng	619669	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	94
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
5	1-Hexadecanol	242	C16H34O	036653-82-4	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

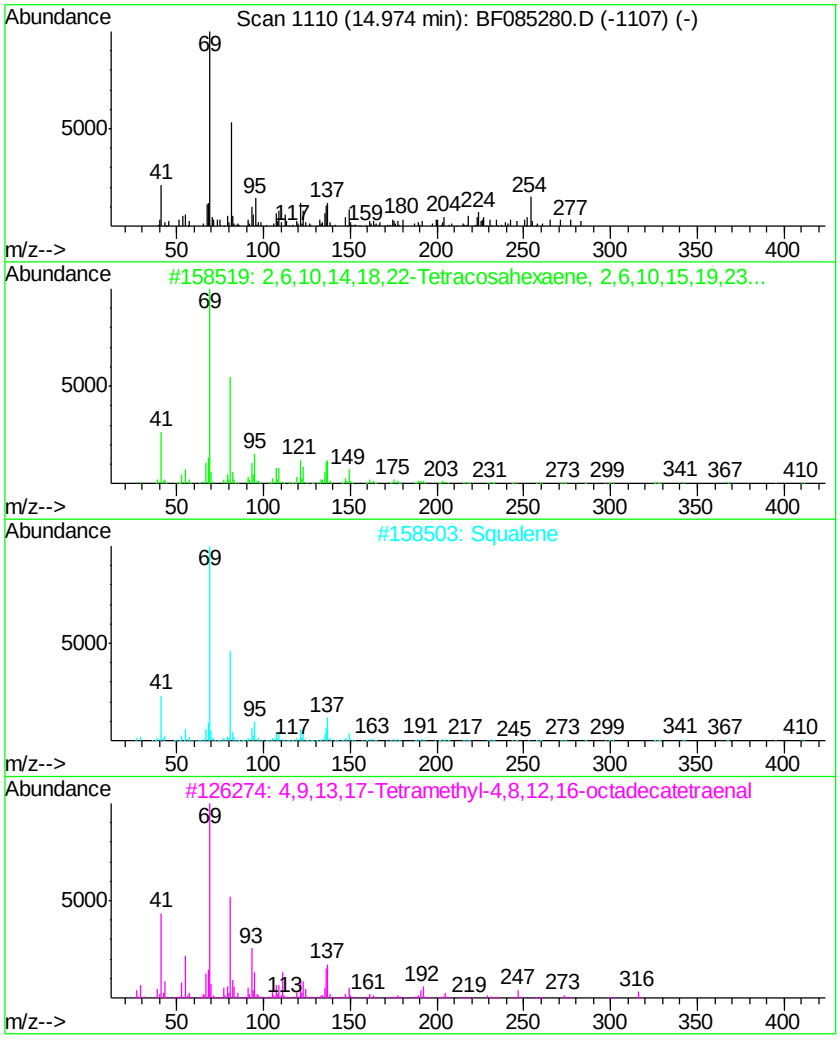
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

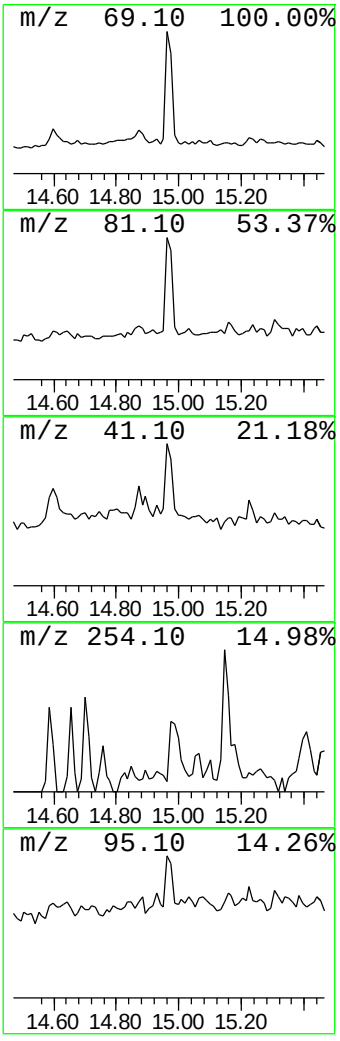
****

Peak Number 9 2,6,10,14,18,22-Tetracosahe... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.20 ng	99168	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	81
2	Squalene	410	C30H50	007683-64-9	74
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

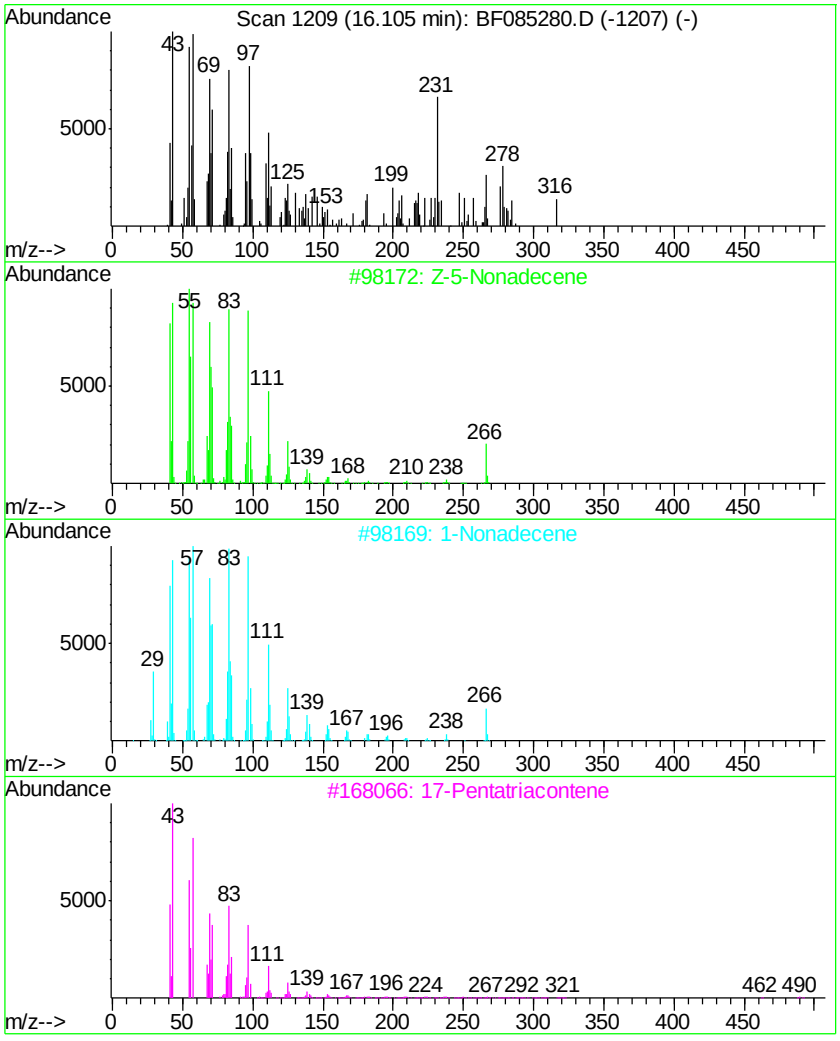
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

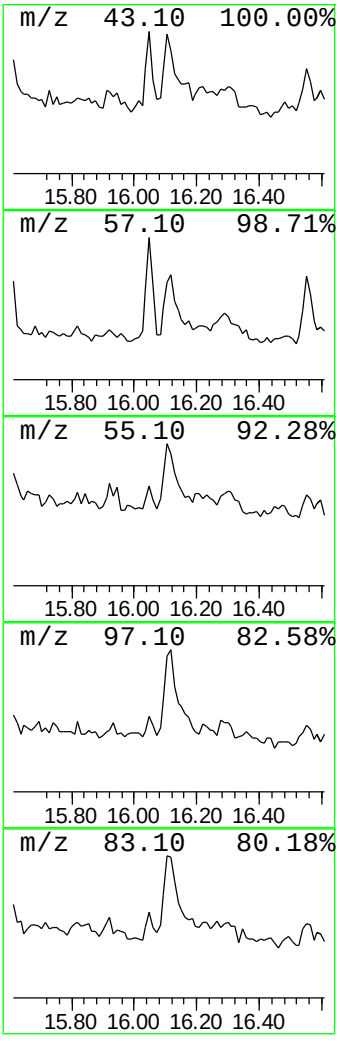
****

Peak Number 11 Z-5-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	3.49 ng	157372	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	76
2	1-Nonadecene	266	C19H38	018435-45-5	68
3	17-Pentatriacontene	491	C35H70	006971-40-0	68
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	64
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	62





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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

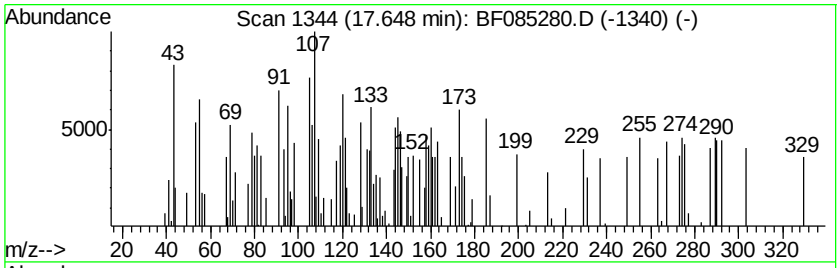
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

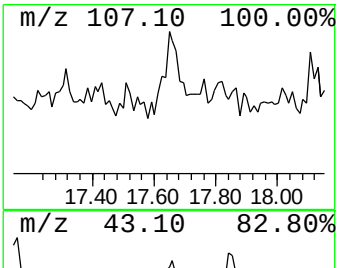
****

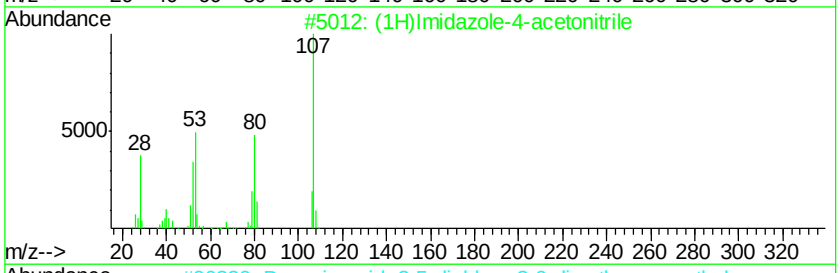
Peak Number 12 unknown17.65 Concentration Rank 13

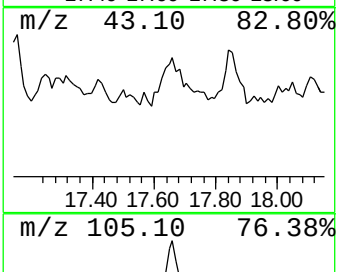
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.65	2.04 ng	92049	Perylene-d12	15.58

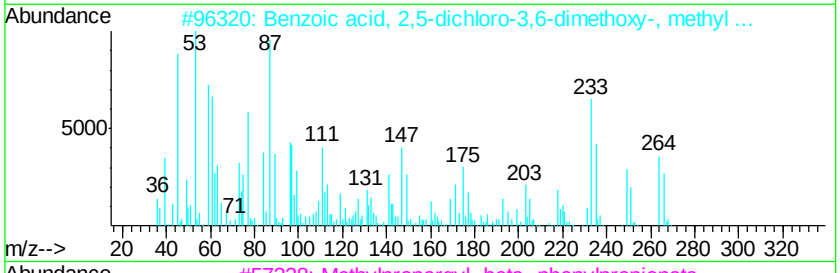
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1H)Imidazole-4-acetonitrile	107	C5H5N3	018502-05-1	25
2	Benzoic acid, 2,5-dichloro-3,6-d...	264	C10H10Cl2O4	062059-39-6	20
3	Methylpropargyl-.beta.-phenylpro...	202	C13H14O2	028048-99-9	13
4	1-Pentyn-3-one, 4-methyl-	96	C6H8O	013531-82-3	10
5	6-Aminotetrazolo(b)pyridazine	136	C4H4N6	019195-43-8	10

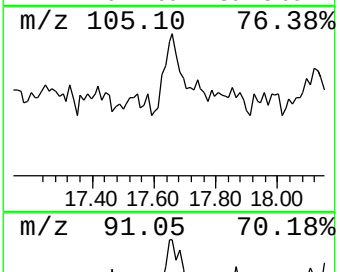


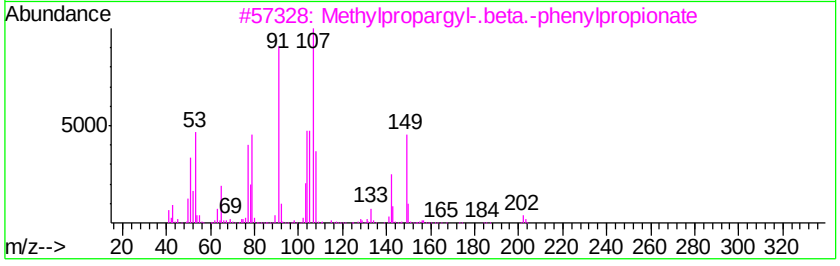


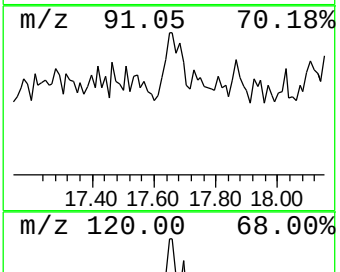


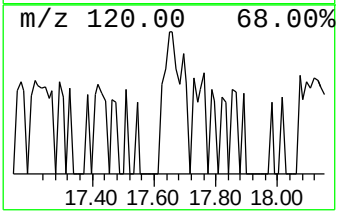












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085280.D
Acq On : 9 Mar 2016 2:47
Operator : UM/SJ
Sample : H1703-04
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-39COMP(0.5-2.0)

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...	5.17	24.1	ng	1156410	1	6.96	957621	20.0
unknown6.72	6.72	87.7	ng	4200950	1	6.96	957621	20.0
Heptadecane	10.42	2.5	ng	157730	3	10.00	1247180	20.0
n-Hexadecanoic acid	12.00	6.6	ng	486854	4	11.49	1479900	20.0
Octadecanoic acid	12.79	4.4	ng	322952	4	11.49	1479900	20.0
Cyclopentadecane	13.96	8.6	ng	619669	5	14.12	1434630	20.0
2,6,10,14,18,22-T...	14.97	2.2	ng	99168	6	15.58	902396	20.0
Z-5-Nonadecene	16.11	3.5	ng	157372	6	15.58	902396	20.0
unknown17.65	17.65	2.0	ng	92049	6	15.58	902396	20.0