LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

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-BF012417.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	5.161	265	269	275	rVB	1204153	1883503	39.11%	4.520%
2	5.561	301	304	307	rBV	3670691	3968308	82.39%	9.523%
3	6.590	390	394	396	rBV	3918261	4816360	100.00%	11.558%
4	6.727	403	406	409	rBV	3299388	4125191	85.65%	9.899%
5	6.967	425	427	429	rBV	1123104	974697	20.24%	2.339%
6	7.127	438	441	443	rBV	3252902	3367629	69.92%	8.081%
7	7.527	473	476	479	rBV	2168719	2642057	54.86%	6.340%
8	8.259	537	540	542	rBV	1503713	1346184	27.95%	3.230%
9	9.345	632	635	637	rBV	4426765	4428388	91.94%	10.627%
10	9.733	667	669	671	rBV	331998	304067	6.31%	0.730%
11	9.962	687	689	691	rVB	54107	55461	1.15%	0.133%
12	10.019	692	694	696	rVB	1184018	1396500	28.99%	3.351%
13	10.465	729	733	734	rBV	104976	133095	2.76%	0.319%
14	10.682	749	752	755	rBV	48463	72708	1.51%	0.174%
15	10.819	761	764	766	rBV	2076080	2581863	53.61%	6.196%
16	10.933	772	774	779	rVB	178218	206132	4.28%	0.495%
17	11.390	811	814	815	rBV	83005	118403	2.46%	0.284%
18	11.516	822	825	826	rBV	1478299	1439939	29.90%	3.455%
19	11.813	849	851	853	rBV	70933	60762	1.26%	0.146%
20	12.042	869	871	876	rVB	185414	190921	3.96%	0.458%
21	12.728	928	931	932	rBV	109648	114114	2.37%	0.274%
22	12.831	937	940	943	rVV2	36767	48279	1.00%	0.116%
23	12.956	947	951	952	rBV	100315	136648	2.84%	0.328%
24	12.979	952	953	958	rVB	90353	91217	1.89%	0.219%
25	13.105	961	964	967	rBV	3876811	3862673	80.20%	9.269%
26	13.334	983	984	987	rVB	69863	79042	1.64%	0.190%
27	13.676	1012	1014	1018	rVB	67400	72380	1.50%	0.174%
28	13.996	1040	1042	1048	rBV	289104	330706	6.87%	0.794%
29	14.145	1052	1055	1058	rBV	936952	1315080	27.30%	3.156%
30	14.625	1095	1097	1099	rBV	49062	65232	1.35%	0.157%
31	15.014	1129	1131	1134	rBV	163648	235999	4.90%	0.566%
32	15.197	1144	1147	1152	rVB	30621	79872	1.66%	0.192%
33	15.288	1152	1155	1159	rBV2	46990	75342	1.56%	0.181%
34	15.631	1182	1185	1187	rBV	588261	881341	18.30%	2.115%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

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-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.122	1226	1228	1230	rBV	40831	67879	1.41%	0.163%
36	16.648	1271	1274	1278	rBV2	27817	48362	1.00%	0.116%
37	17.254	1324	1327	1331	rBV	21360	56520	1.17%	0.136%

Sum of corrected areas: 41672854

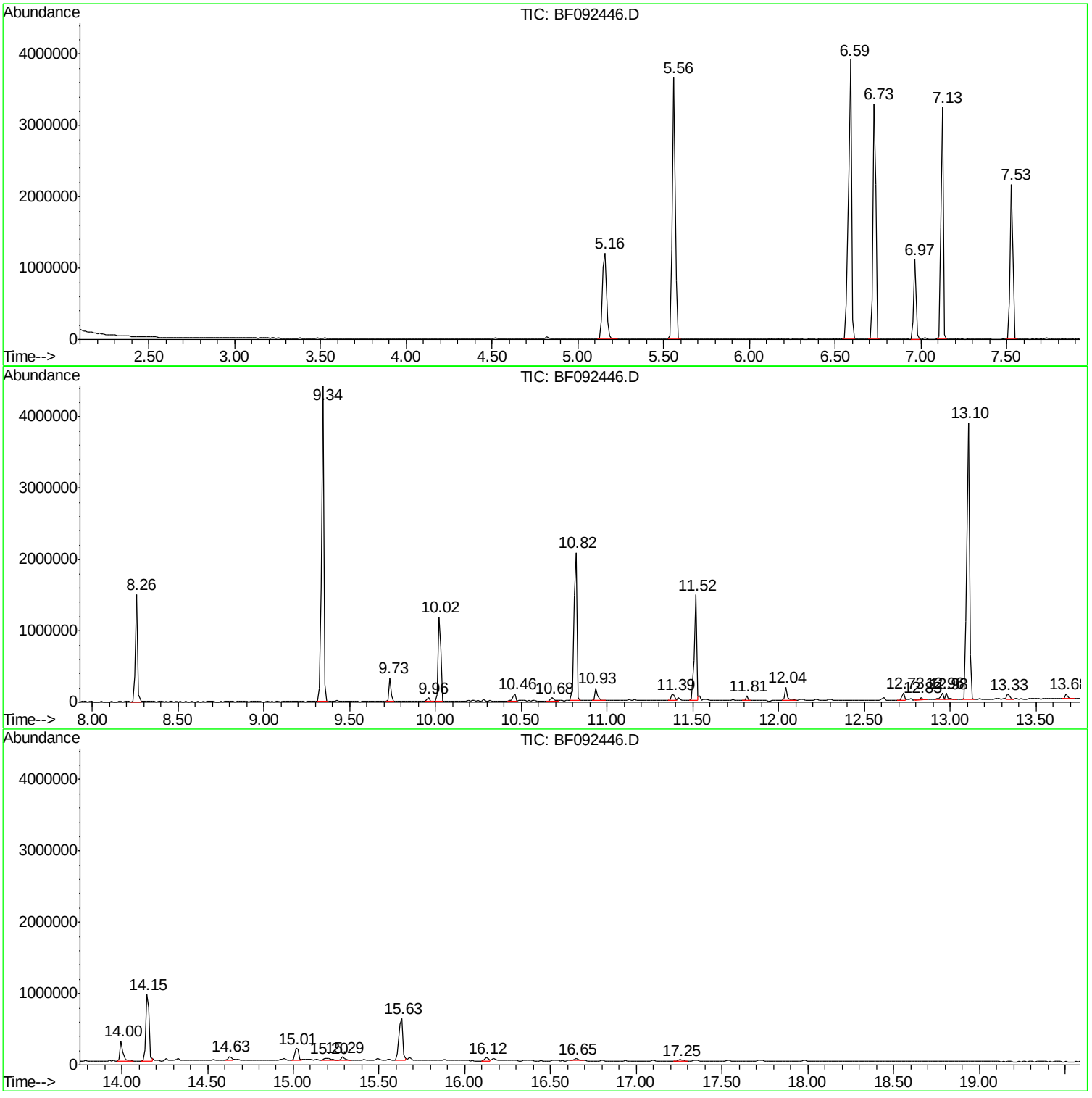
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

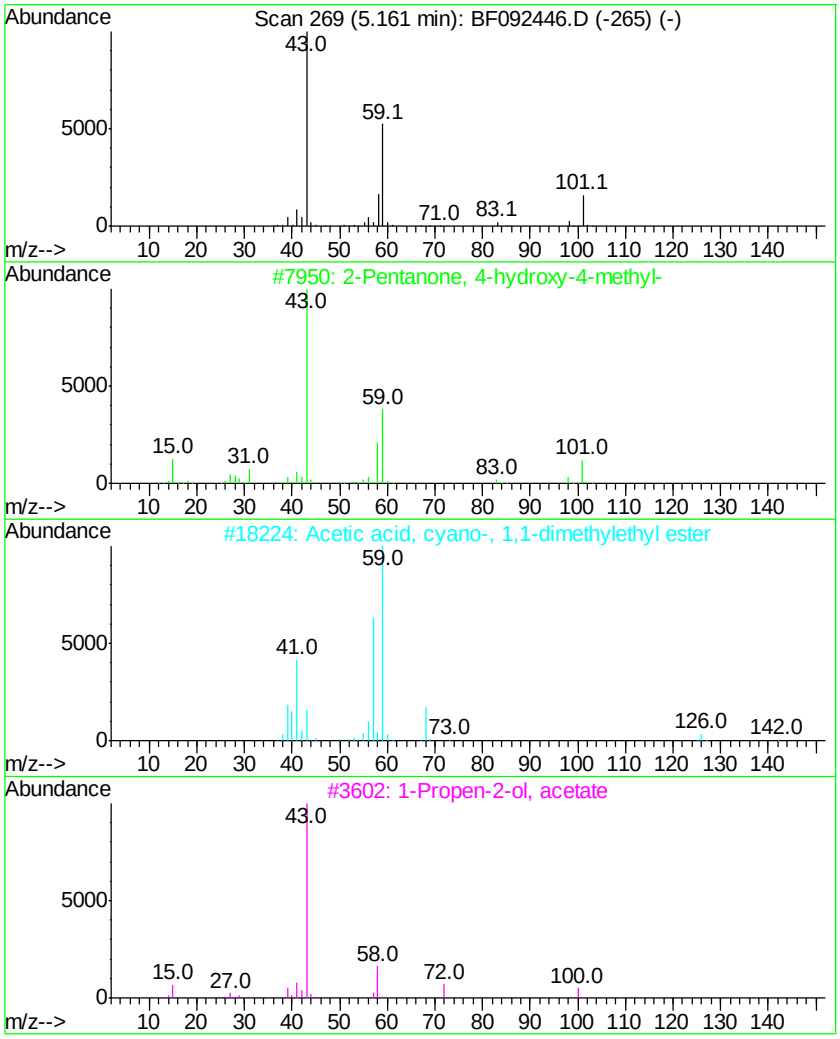
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

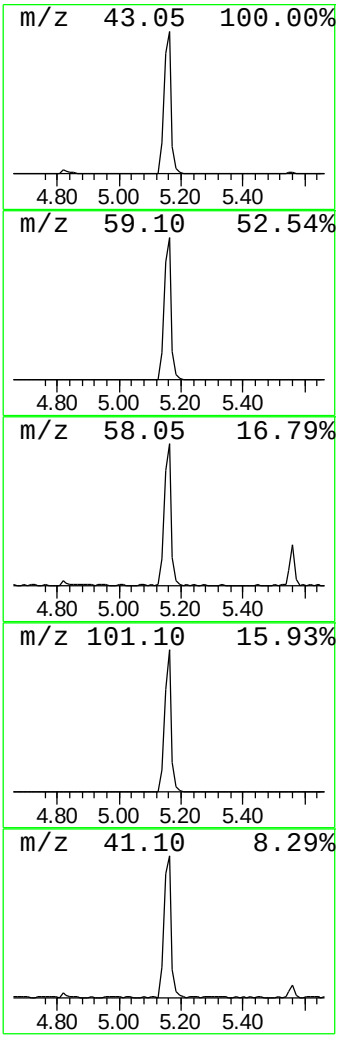
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	38.65 ng	1883500	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

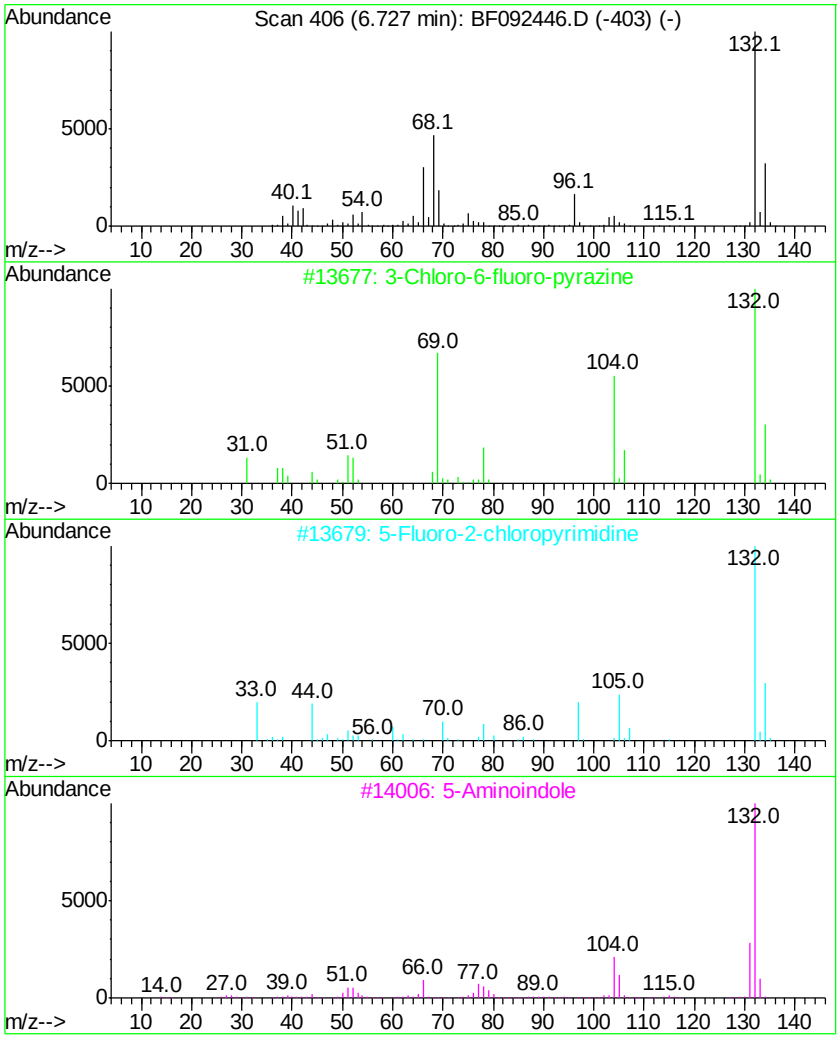
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

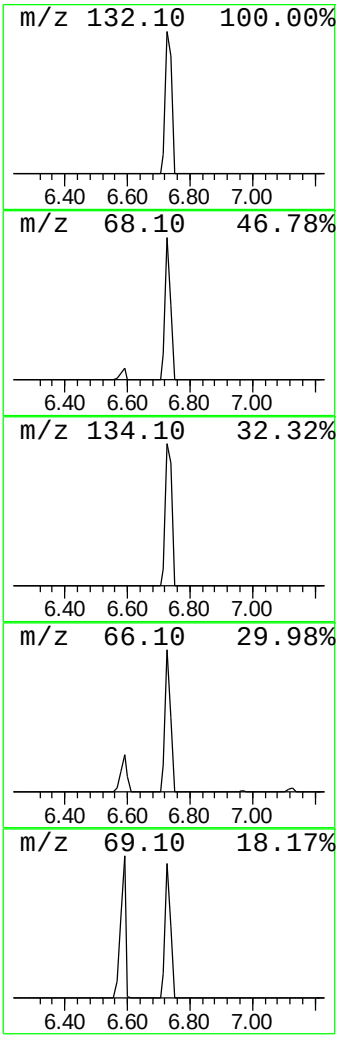
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	84.65 ng	4125190	1,4-Dichlorobenzene-d4	6.97

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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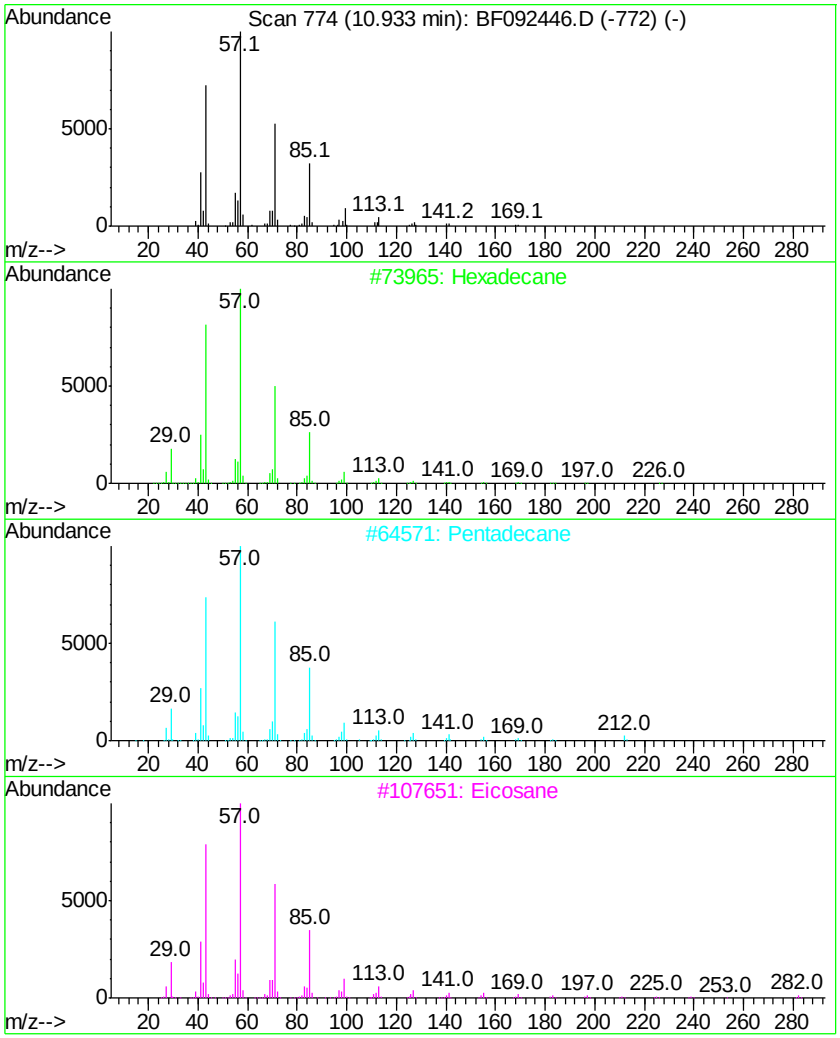
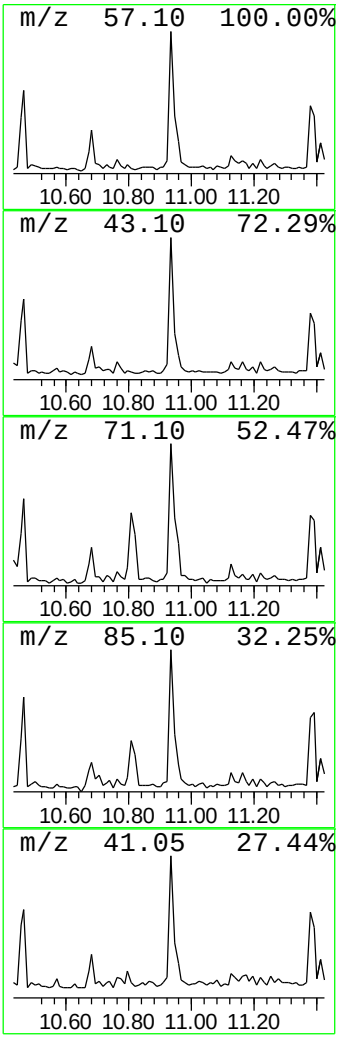
Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	2.86 ng	206132	Phenanthrene-d10	11.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Eicosane	282	C20H42	000112-95-8	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

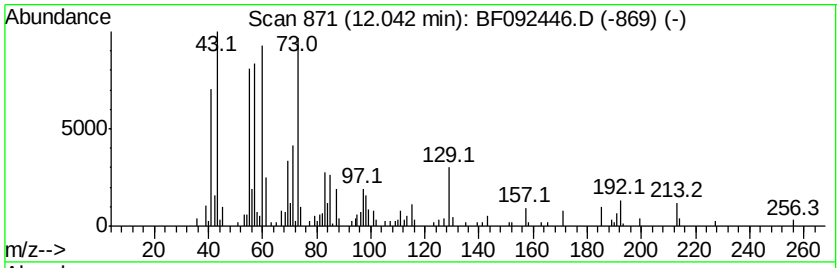
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

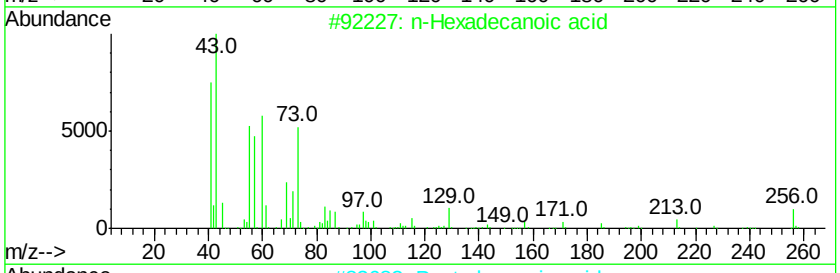
****

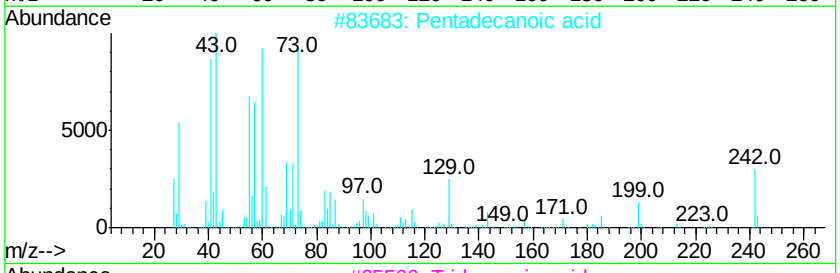
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

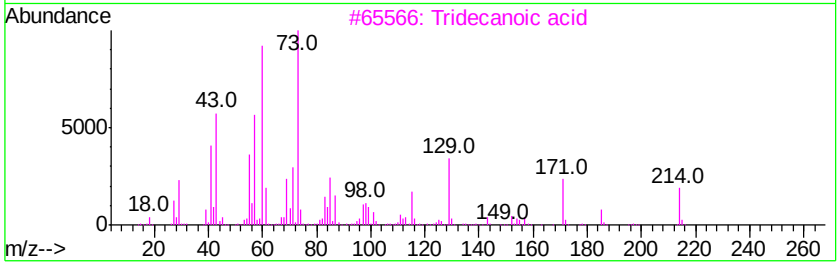
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	2.65 ng	190921	Phenanthrene-d10	11.52

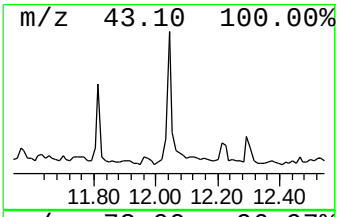
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Tritetracontane	605	C43H88	007098-21-7	11

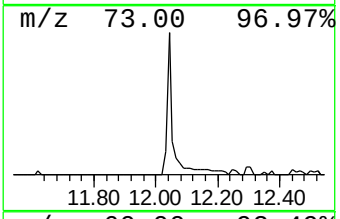


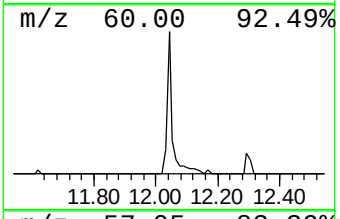


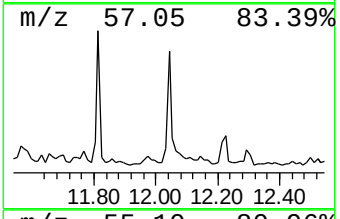


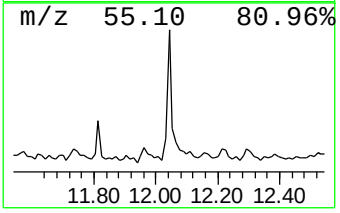












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Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

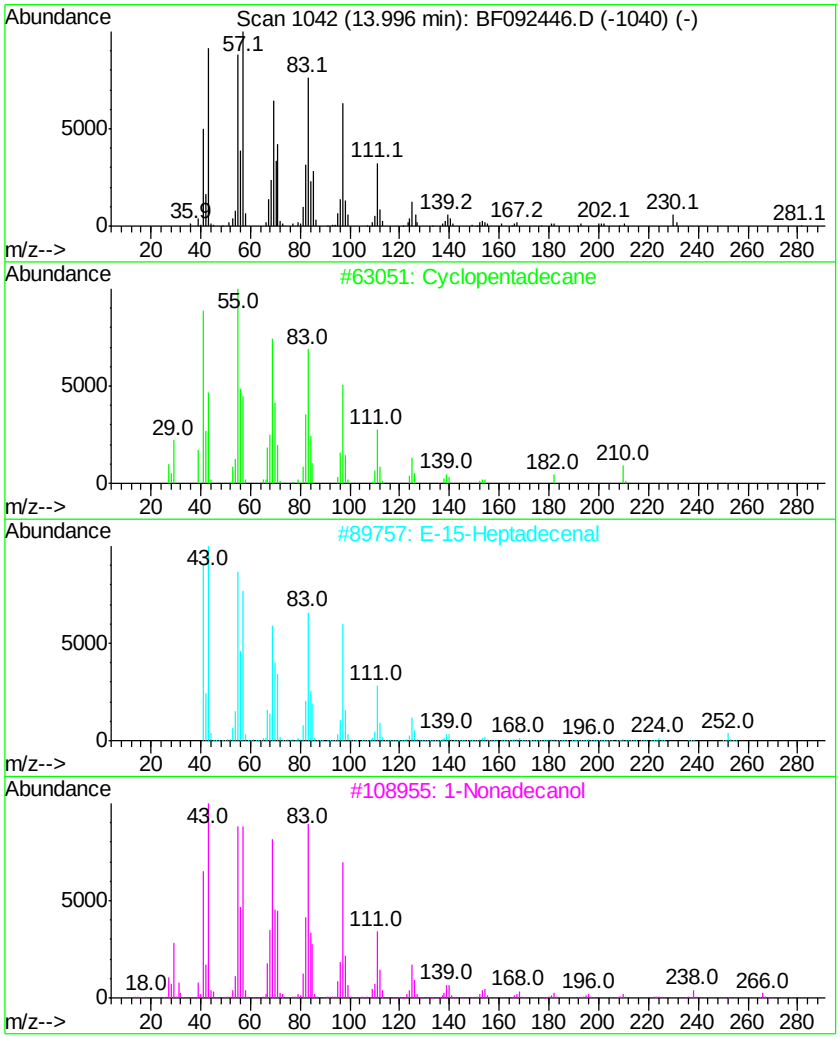
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

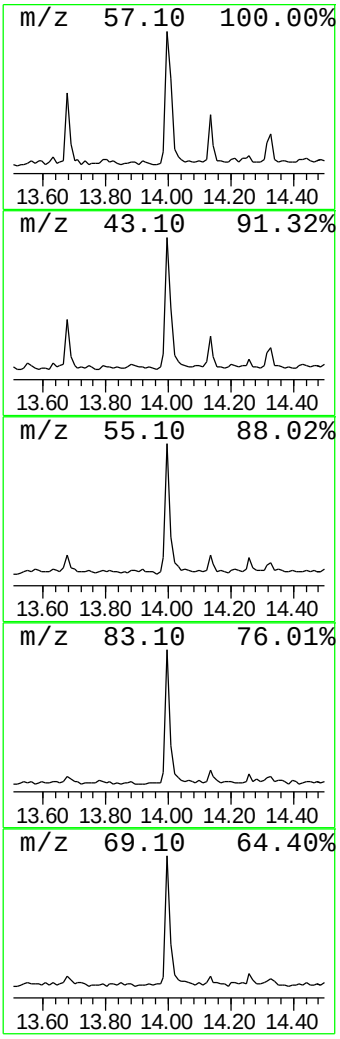
****

Peak Number 7 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	5.03 ng	330706	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
3	1-Nonadecanol	284	C19H40O	001454-84-8	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91





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Sample : I1382-05
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

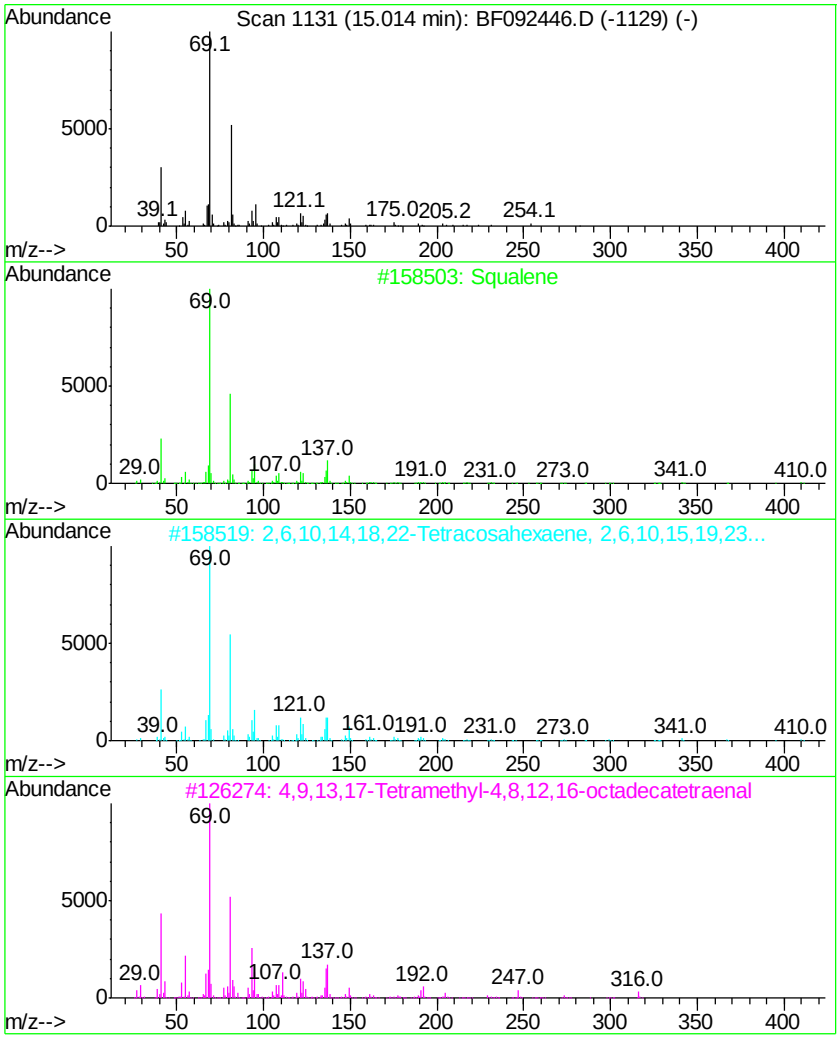
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

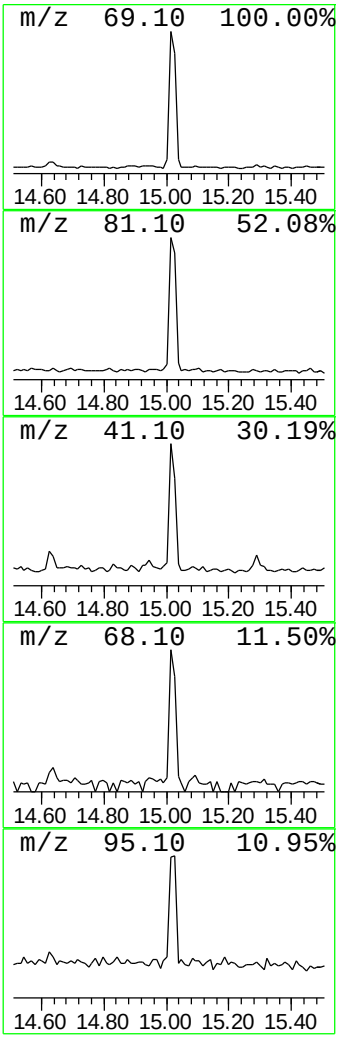
****

Peak Number 8 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	5.36 ng	235999	Perylene-d12	15.63

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	83
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	Propanoic acid, 2,2-dimethyl-, [...	306	C20H34O2	1000164-38-8	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092446.D
Acq On : 24 Jan 2017 23:13
Operator : UM/SJ
Sample : I1382-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-01-001-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.16	38.6	ng	1883500	1	6.97	974697	20.0
unknown6.73	6.73	84.7	ng	4125190	1	6.97	974697	20.0
Hexadecane	10.93	2.9	ng	206132	4	11.52	1439940	20.0
n-Hexadecanoic acid	12.04	2.6	ng	190921	4	11.52	1439940	20.0
Cyclopentadecane	14.00	5.0	ng	330706	5	14.16	1315080	20.0
Squalene	15.01	5.4	ng	235999	6	15.63	881341	20.0