LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-B-20150873

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-BF121315.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	2.190	6	9	28	rVB2	39457	125215	3.81%	0.480%
2	4.418	202	204	210	rVB2	57329	85520	2.60%	0.328%
3	4.887	243	245	249	rVB	41648	40544	1.23%	0.155%
4	5.093	260	263	268	rBV	442976	721805	21.94%	2.767%
5	5.504	296	299	302	rBV	1853389	2430375	73.87%	9.315%
6	6.533	385	389	391	rBV	2204848	2664986	81.01%	10.214%
7	6.659	398	400	403	rBV	2044332	2607035	79.24%	9.992%
8	6.887	418	420	422	rBV	533323	503631	15.31%	1.930%
9	7.047	432	434	437	rVB	2056200	1994454	60.62%	7.644%
10	7.459	466	470	472	rBV	1525412	1862557	56.62%	7.139%
11	8.179	530	533	535	rBV	523597	694779	21.12%	2.663%
12	9.253	624	627	629	rBV	3385969	3289862	100.00%	12.610%
13	9.642	659	661	663	rBV	808022	650080	19.76%	2.492%
14	9.928	683	686	688	rBV	935916	835367	25.39%	3.202%
15	10.362	723	724	726	rVB	44407	37845	1.15%	0.145%
16	10.716	752	755	757	rBV	1969492	1986854	60.39%	7.615%
17	10.830	764	765	770	rVB	38486	69213	2.10%	0.265%
18	11.288	802	805	806	rBV	38382	44096	1.34%	0.169%
19	11.402	813	815	818	rBV	593069	796590	24.21%	3.053%
20	11.631	833	835	838	rBV	101531	138550	4.21%	0.531%
21	12.191	882	884	886	rBV	234508	207655	6.31%	0.796%
22	12.613	919	921	923	rBV	65796	56722	1.72%	0.217%
23	12.842	938	941	943	rBV	52357	50861	1.55%	0.195%
24	12.991	951	954	957	rBV	2573713	2715787	82.55%	10.409%
25	13.882	1030	1032	1036	rBV	84400	106723	3.24%	0.409%
26	14.042	1043	1046	1048	rBV	501245	647792	19.69%	2.483%
27	14.888	1118	1120	1123	rBV	46761	49049	1.49%	0.188%
28	15.059	1133	1135	1140	rVB	20741	49697	1.51%	0.190%
29	15.151	1140	1143	1146	rBV2	20191	44879	1.36%	0.172%
30	15.471	1168	1171	1174	rBV	342457	470166	14.29%	1.802%
31	15.940	1209	1212	1214	rBV	18786	33242	1.01%	0.127%
32	19.483	1517	1522	1527	rVB5	24147	78305	2.38%	0.300%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-B-20150873

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

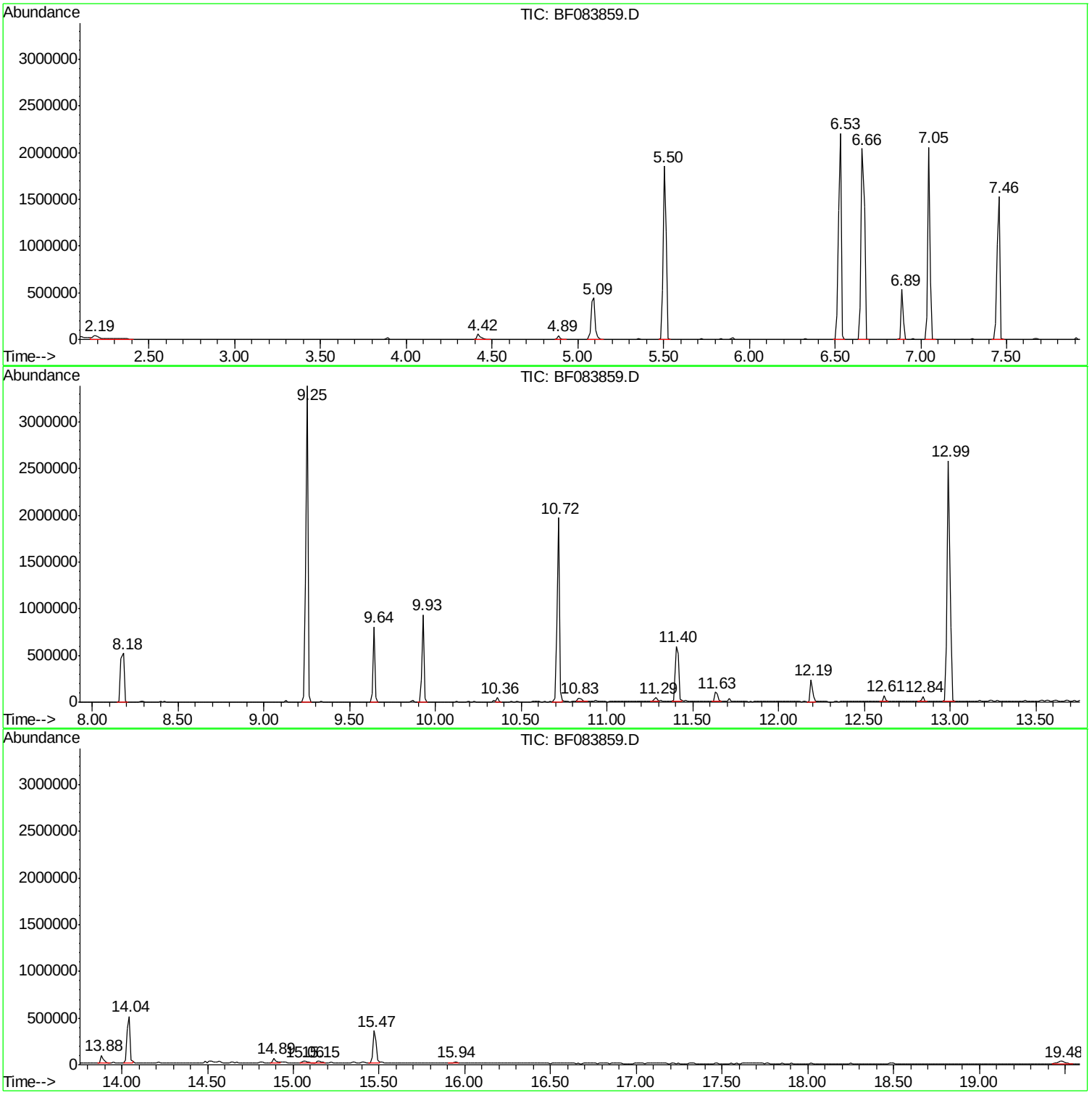
Sum of corrected areas: 26090236

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

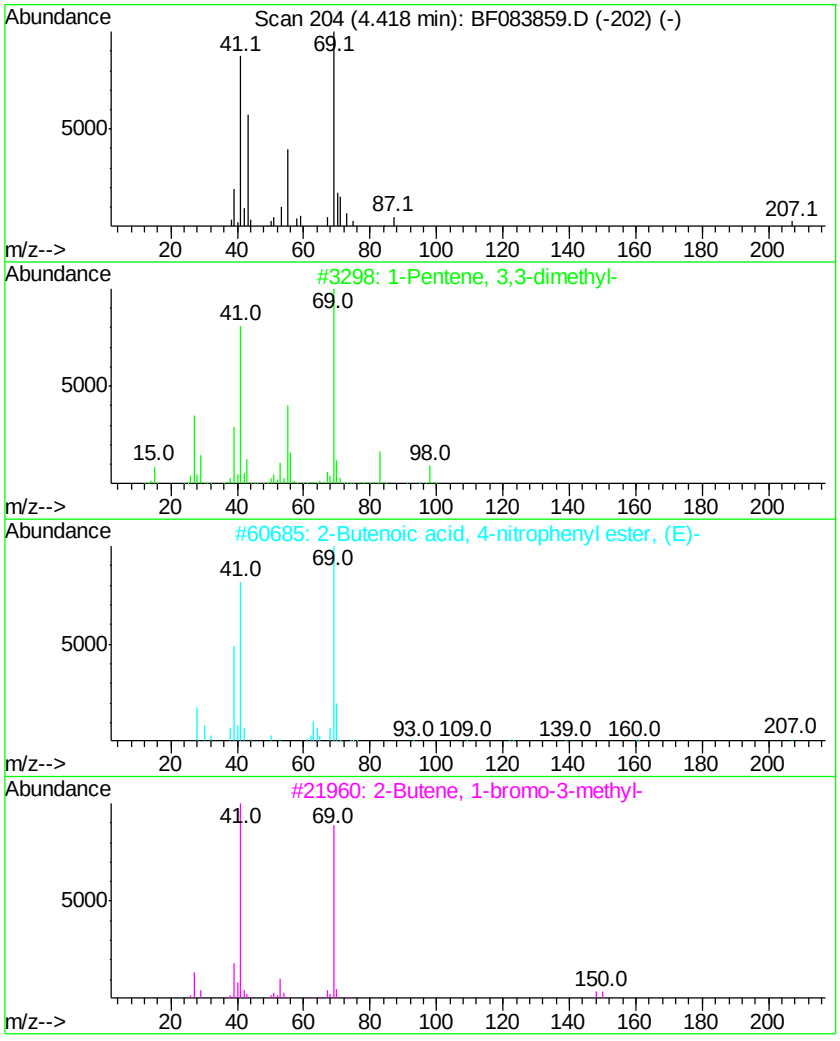
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

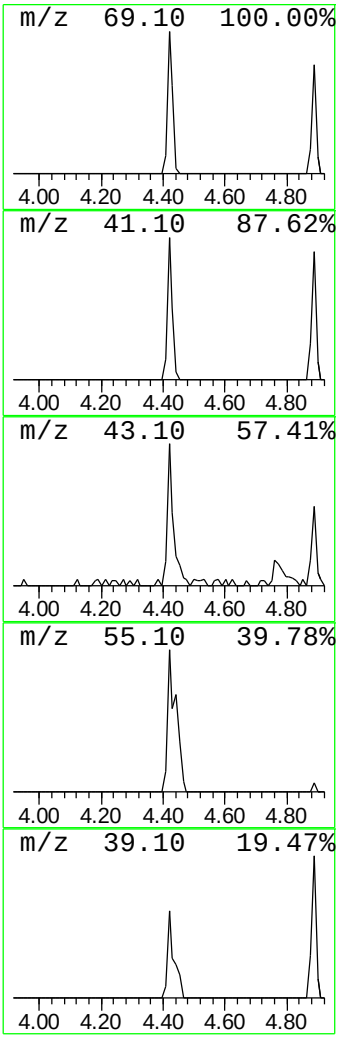
****

Peak Number 2 1-Pentene, 3,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	3.40 ng	85520	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	64
2	2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	59
3	2-Butene, 1-bromo-3-methyl-	148	C5H9Br	000870-63-3	42
4	1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	38
5	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

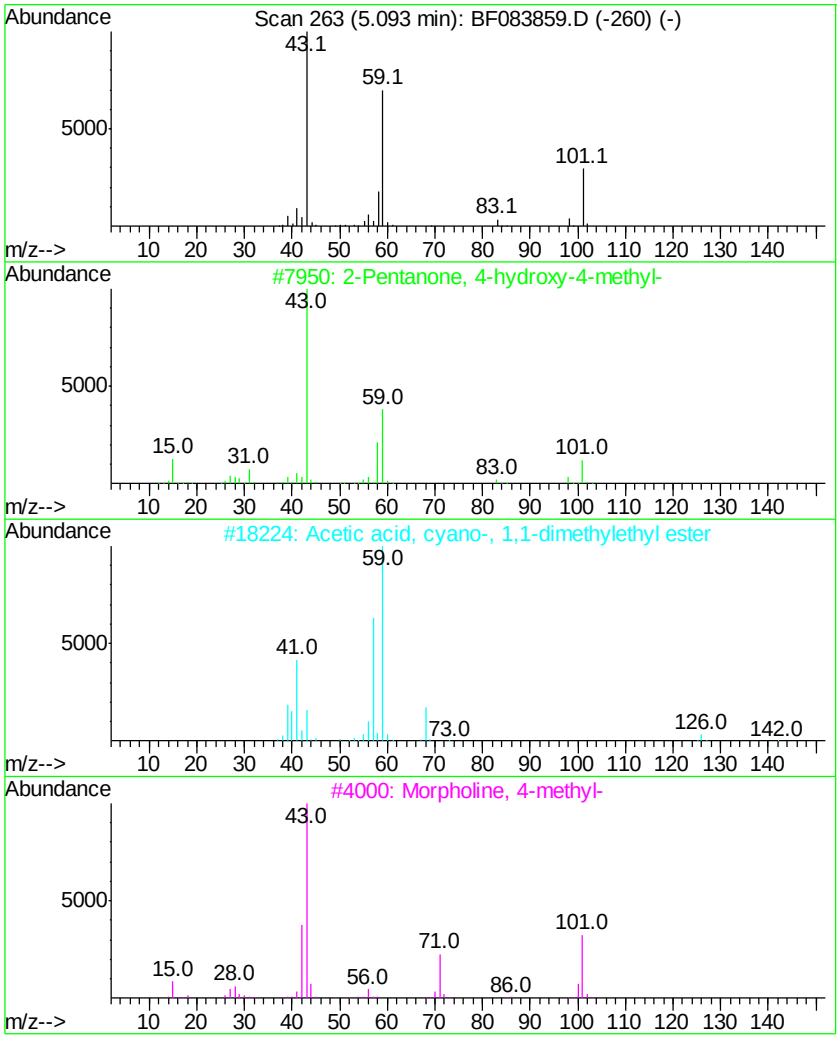
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

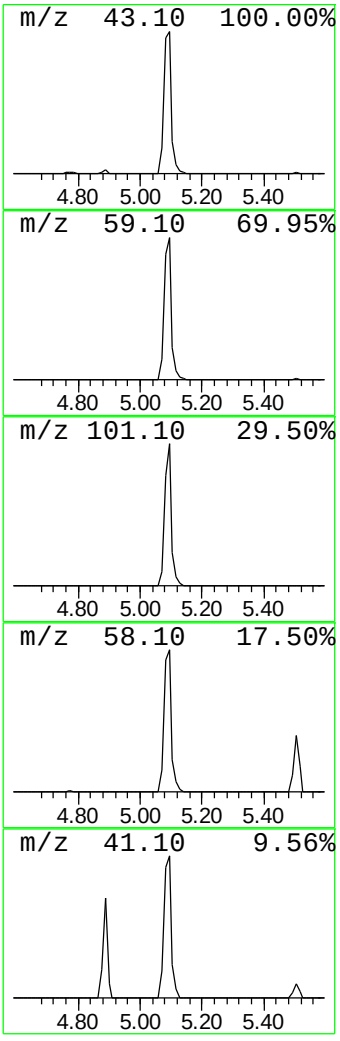
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	28.66 ng	721805	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

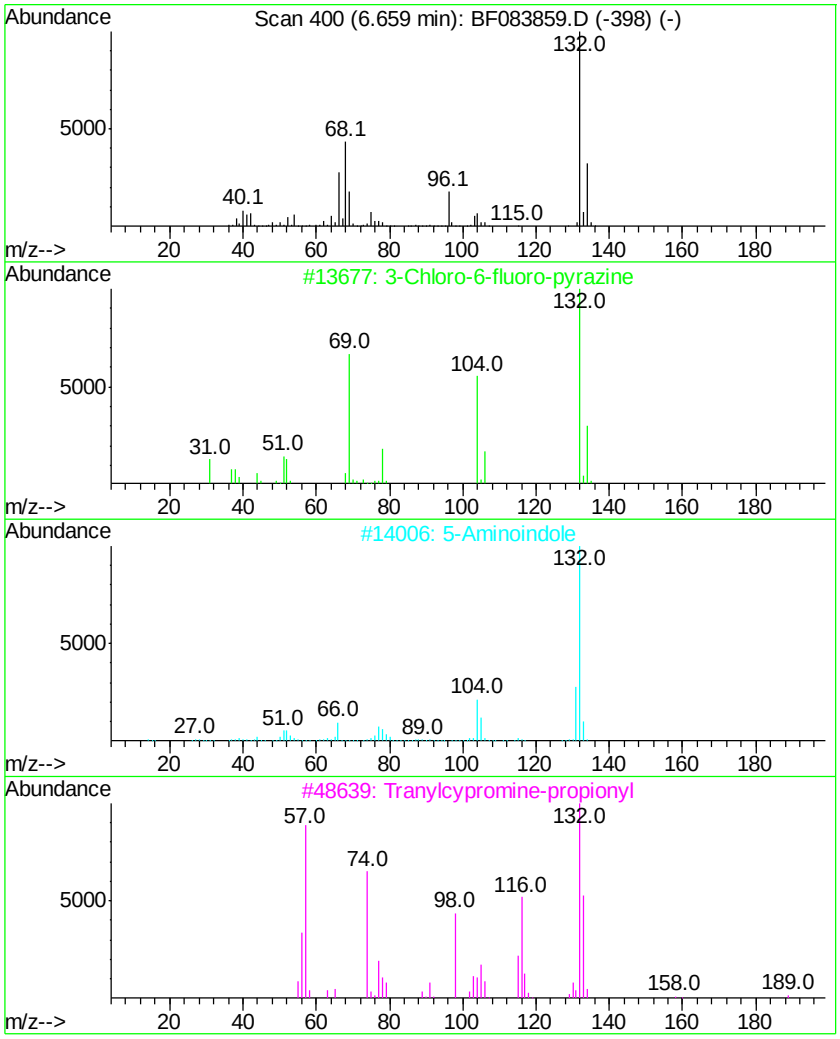
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

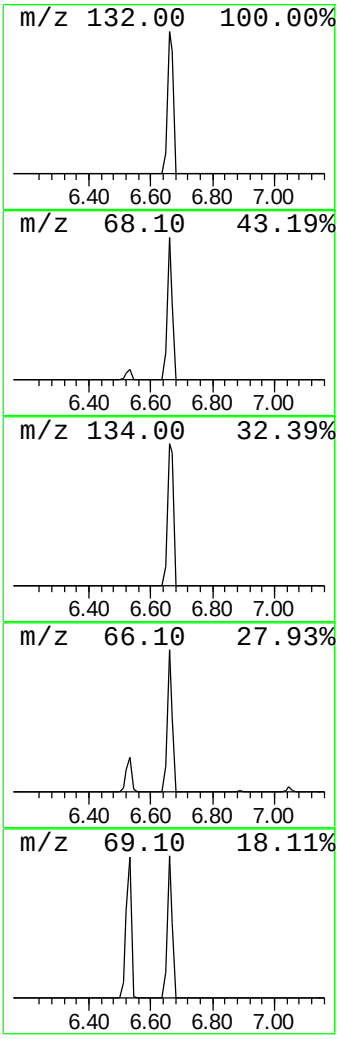
****

Peak Number 4 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	103.53 ng	2607040	1,4-Dichlorobenzene-d4	6.89

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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

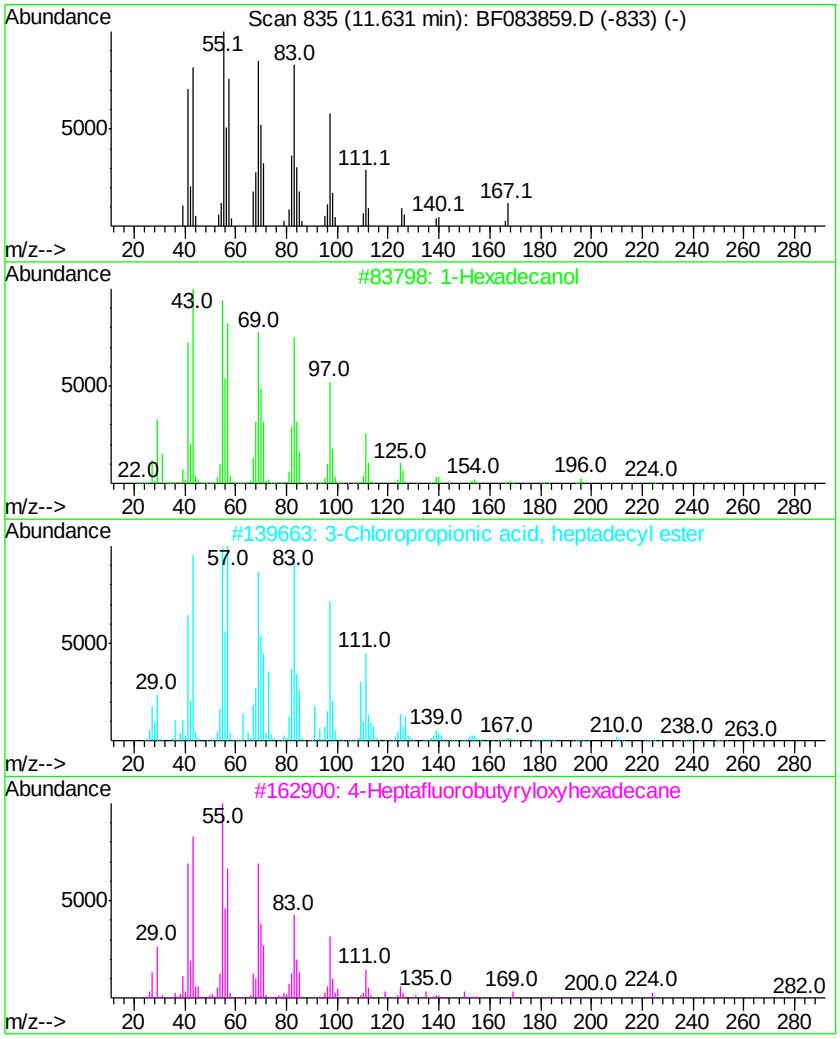
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

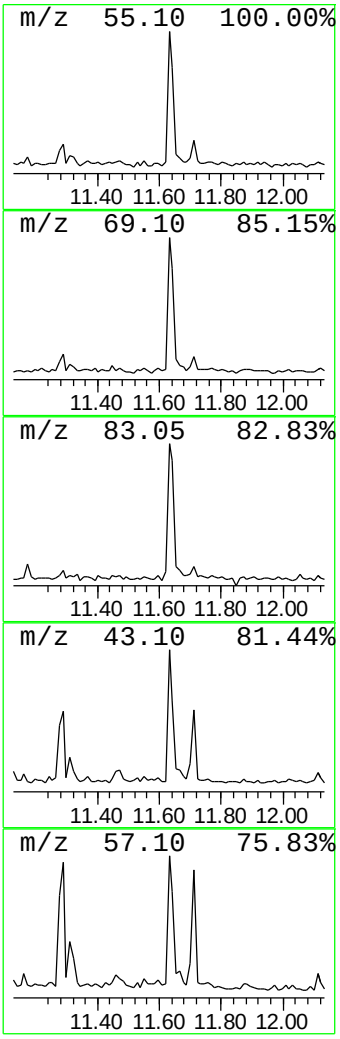
****

Peak Number 6 1-Hexadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	3.48 ng	138550	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
4	1-Heptadecanol	256	C17H36O	001454-85-9	90
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

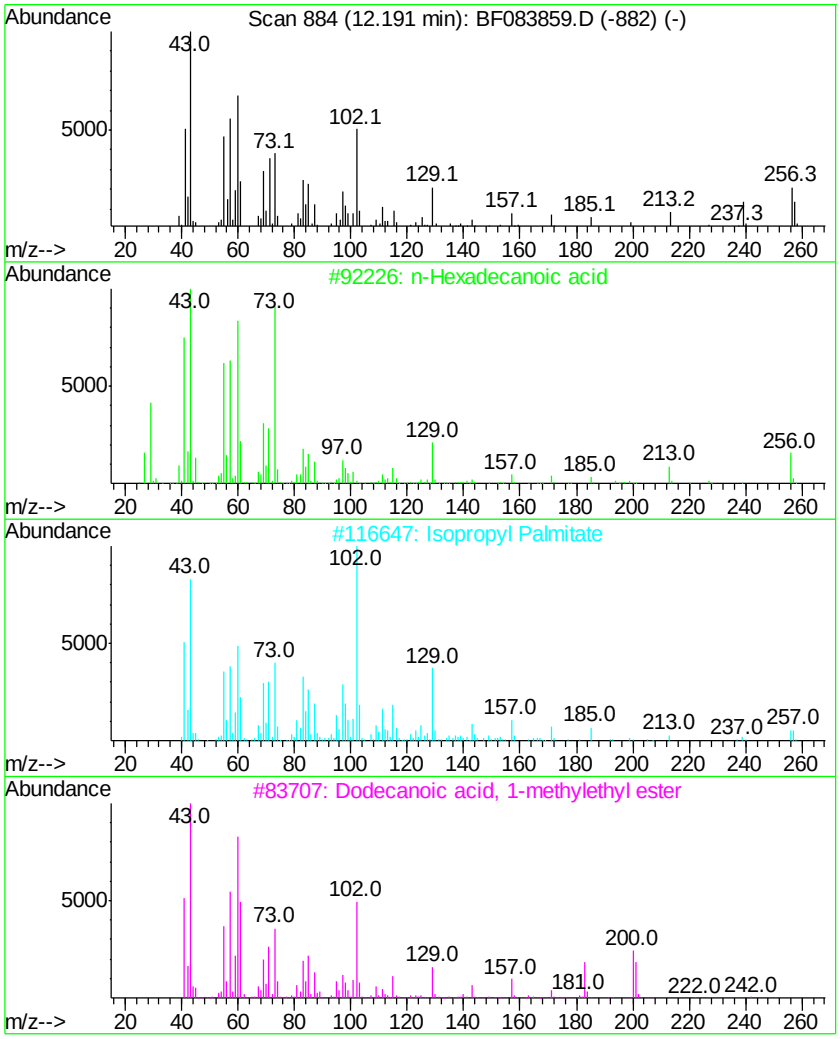
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

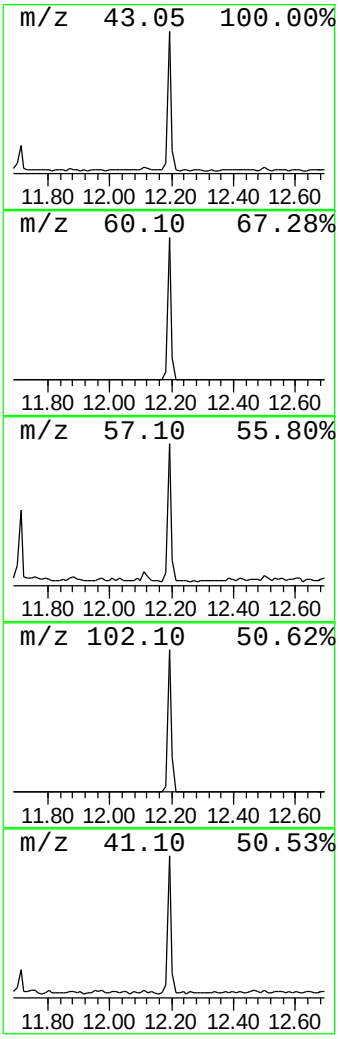
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.19	5.21 ng	207655	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
2	Isopropyl Palmitate	298	C19H38O2	000142-91-6	49
3	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	47
4	Isopropyl Myristate	270	C17H34O2	000110-27-0	47
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30





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Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
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Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

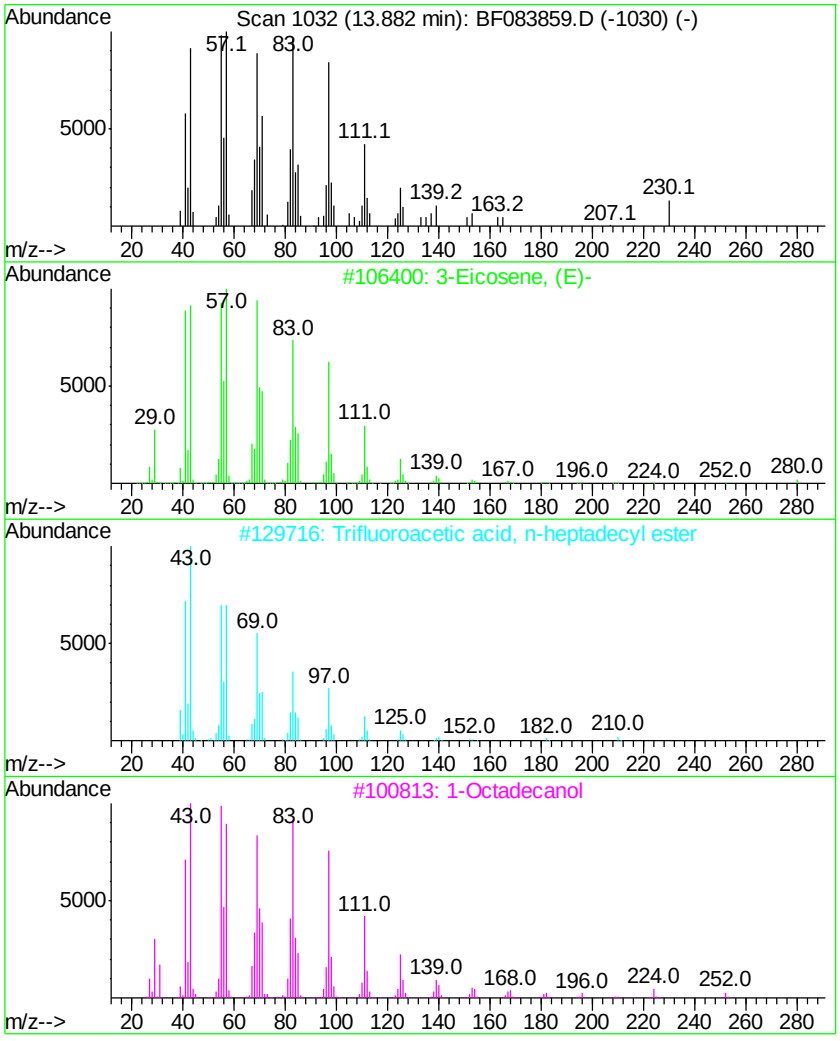
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

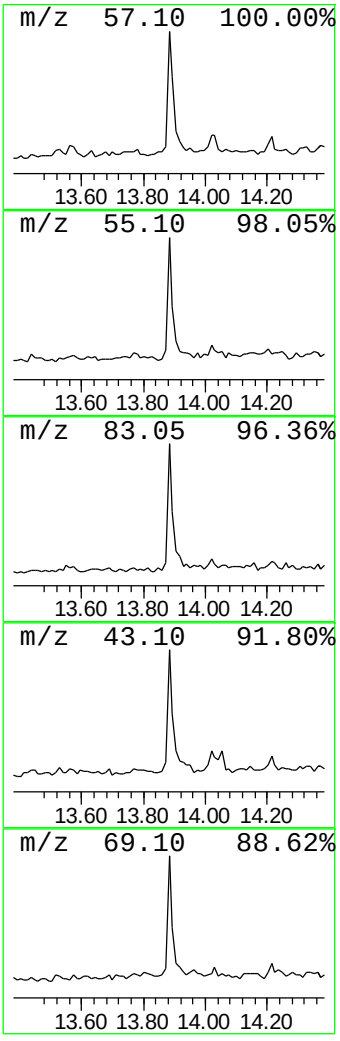
****

Peak Number 8 3-Eicosene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.29 ng	106723	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	11-Tricosene	322	C23H46	052078-56-5	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

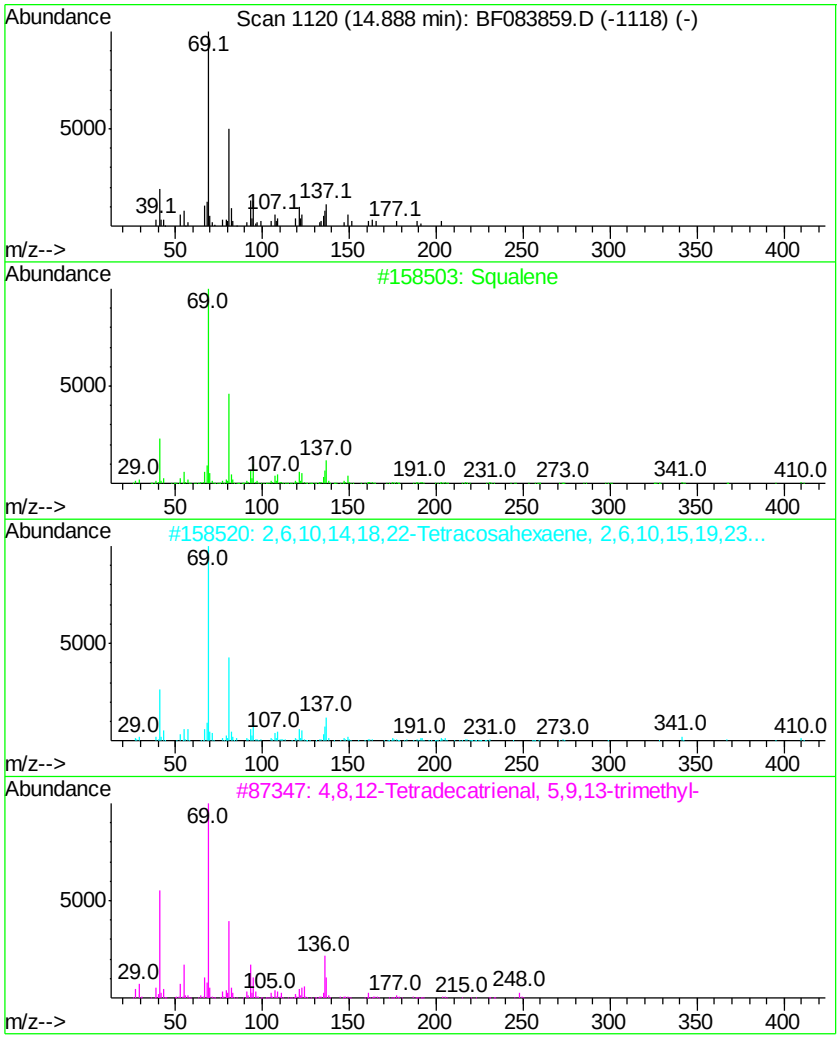
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

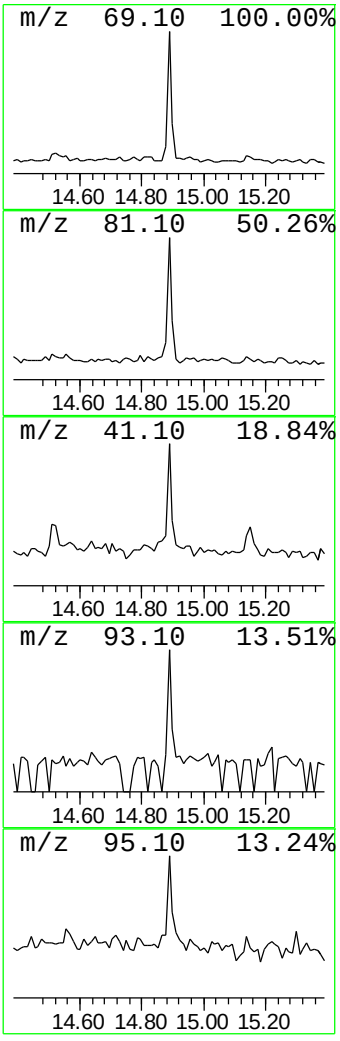
****

Peak Number 9 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.09 ng	49049	Perylene-d12	15.47

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	86
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64





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Data File : BF083859.D
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Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

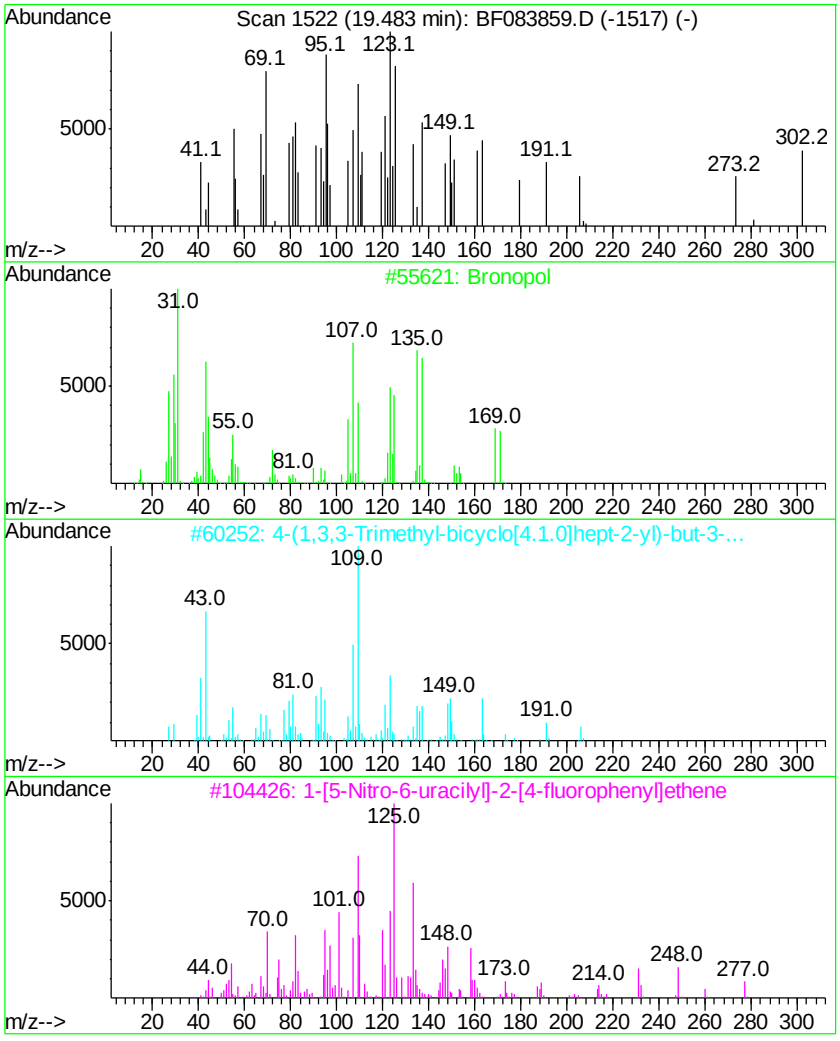
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

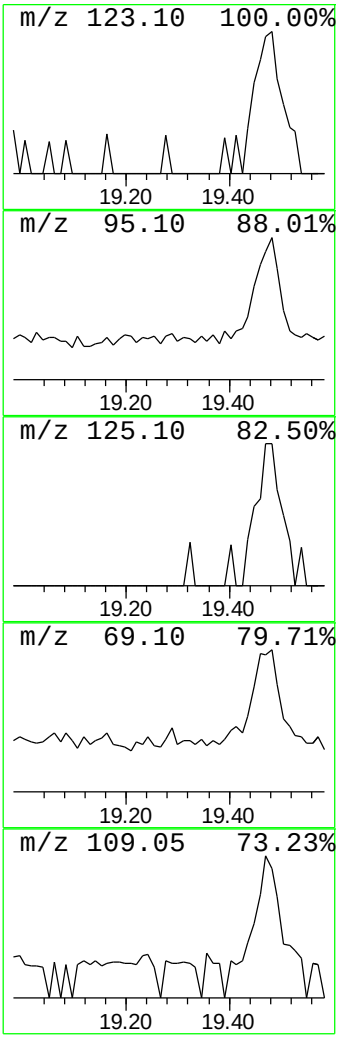
****

Peak Number 11 unknown19.48 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.48	3.33 ng	78305	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bronopol	199	C3H6BrNO4	000052-51-7	25
2	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	25
3	1-[5-Nitro-6-uracilyl]-2-[4-fluo...	277	C12H8FN3O4	343354-75-6	22
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	16
5	(4R*,5R*,9S*)-5,9-Dimethylspiro[...	166	C11H18O	063088-19-7	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121615\
Data File : BF083859.D
Acq On : 16 Dec 2015 20:21
Operator : UM/SJ
Sample : G4775-13
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-B-20150873

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.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
1-Pentene, 3,3-di...	4.42	3.4	ng	85520	1	6.89	503631	20.0
2-Pentanone, 4-hy...	5.09	28.7	ng	721805	1	6.89	503631	20.0
unknown6.66	6.66	103.5	ng	2607040	1	6.89	503631	20.0
1-Hexadecanol	11.63	3.5	ng	138550	4	11.41	796590	20.0
n-Hexadecanoic acid	12.19	5.2	ng	207655	4	11.41	796590	20.0
3-Eicosene, (E)-	13.88	3.3	ng	106723	5	14.04	647792	20.0
Squalene	14.89	2.1	ng	49049	6	15.47	470166	20.0
unknown19.48	19.48	3.3	ng	78305	6	15.47	470166	20.0