LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-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-BF070117.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	4.875	469	474	482	rVB	350671	508173	20.48%	2.036%
2	5.298	541	546	549	rBV	2509578	2456070	99.00%	9.839%
3	6.322	715	720	723	rBV	2419187	2480904	100.00%	9.939%
4	6.451	737	742	745	rBV	2548410	2434064	98.11%	9.751%
5	6.681	777	781	785	rBV	816403	663810	26.76%	2.659%
6	6.840	803	808	811	rBV	1959088	1736665	70.00%	6.957%
7	7.239	871	876	880	rBV	1440871	1564282	63.05%	6.267%
8	7.340	888	893	898	rVB5	17156	25111	1.01%	0.101%
9	7.963	995	999	1003	rBV	1011565	919922	37.08%	3.685%
10	8.263	1045	1050	1053	rVB4	19303	28086	1.13%	0.113%
11	8.404	1070	1074	1078	rBV	138289	137932	5.56%	0.553%
12	8.769	1134	1136	1141	rVB4	19730	27070	1.09%	0.108%
13	8.881	1153	1155	1159	rVB3	31984	31029	1.25%	0.124%
14	9.004	1171	1176	1178	rBV	188372	193891	7.82%	0.777%
15	9.039	1178	1182	1185	rVB	2304846	2215806	89.31%	8.877%
16	9.122	1192	1196	1200	rBV5	53018	70682	2.85%	0.283%
17	9.298	1221	1226	1229	rBV3	29227	51843	2.09%	0.208%
18	9.433	1245	1249	1251	rBV	357872	320762	12.93%	1.285%
19	9.457	1251	1253	1255	rVB	272590	207695	8.37%	0.832%
20	9.610	1273	1279	1280	rBV6	21873	39763	1.60%	0.159%
21	9.633	1280	1283	1286	rVB3	51438	47732	1.92%	0.191%
22	9.663	1286	1288	1291	rBV3	26447	26858	1.08%	0.108%
23	9.716	1291	1297	1300	rBV	960341	1017099	41.00%	4.075%
24	9.886	1320	1326	1328	rBV5	27567	44869	1.81%	0.180%
25	9.922	1329	1332	1335	rVB2	72767	75200	3.03%	0.301%
26	9.986	1340	1343	1347	rBV2	71847	64374	2.59%	0.258%
27	10.092	1357	1361	1362	rBV3	20507	26296	1.06%	0.105%
28	10.280	1391	1393	1397	rVB3	29901	33446	1.35%	0.134%
29	10.380	1406	1410	1414	rBV	311074	306183	12.34%	1.227%
30	10.498	1425	1430	1434	rBV	1501424	1461511	58.91%	5.855%
31	10.645	1450	1455	1462	rBV	602883	642620	25.90%	2.574%
32	10.828	1483	1486	1489	rBV3	36231	49244	1.98%	0.197%
33	10.857	1489	1491	1494	rVB2	47318	45431	1.83%	0.182%
34	11.080	1526	1529	1531	rBV	42506	48505	1.96%	0.194%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.110	1531	1534	1538	rVB	377099	352580	14.21%	1.412%
36	11.192	1543	1548	1551	rBV	1058299	948900	38.25%	3.801%
37	11.457	1590	1593	1597	rVB	68044	73028	2.94%	0.293%
38	11.551	1606	1609	1614	rVB6	22459	25322	1.02%	0.101%
39	11.733	1636	1640	1642	rBV3	32983	35315	1.42%	0.141%
40	11.827	1654	1656	1661	rVB2	33336	32653	1.32%	0.131%
41	12.192	1715	1718	1723	rVB4	22512	28357	1.14%	0.114%
42	12.774	1812	1817	1821	rBV	1966086	1937448	78.09%	7.762%
43	13.680	1966	1971	1977	rBV	127906	136640	5.51%	0.547%
44	13.816	1990	1994	1998	rBV	837721	765598	30.86%	3.067%
45	14.674	2136	2140	2144	rBV	61267	61740	2.49%	0.247%
46	15.210	2227	2231	2238	rBV	450323	561223	22.62%	2.248%

Sum of corrected areas: 24961732

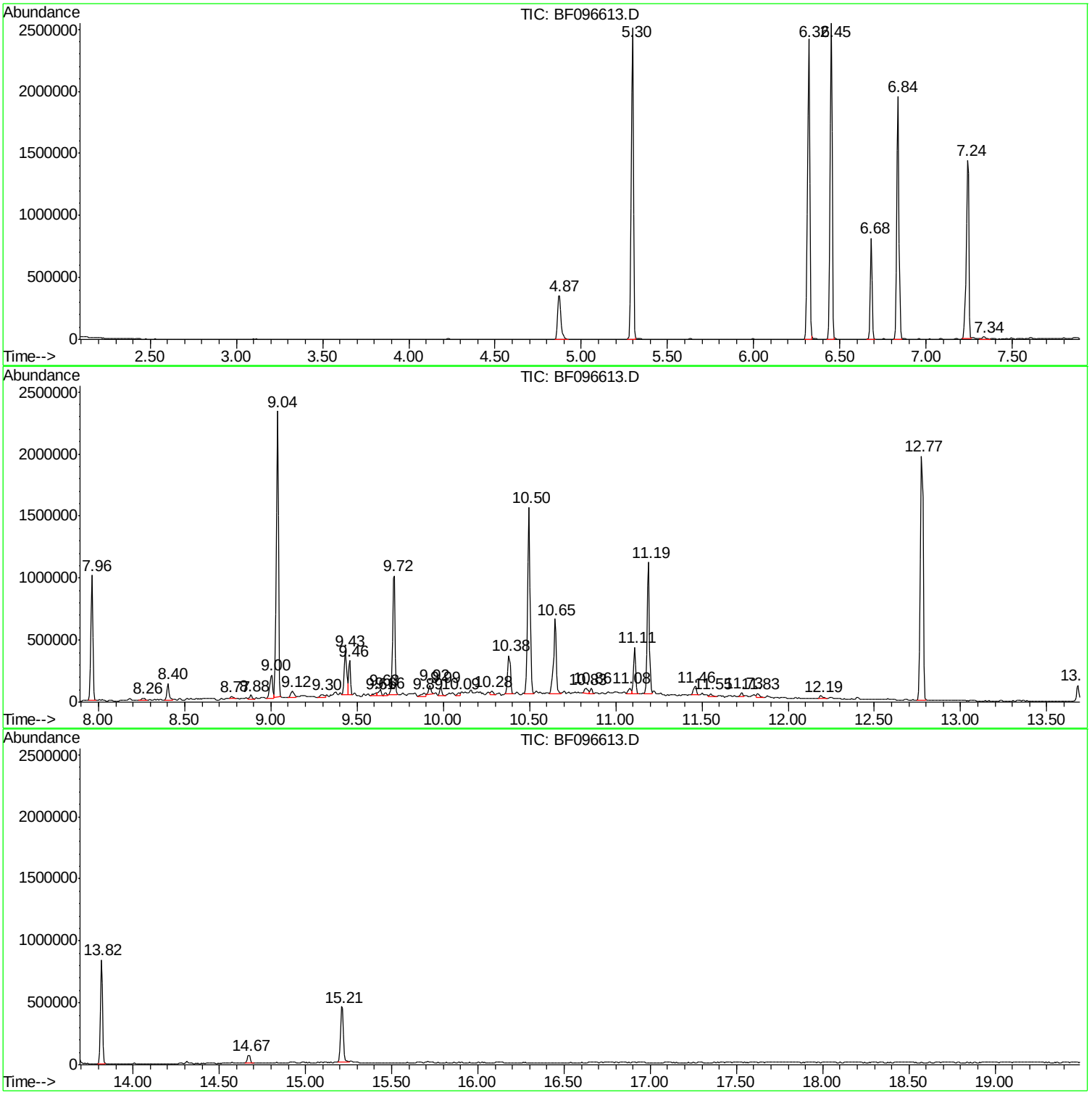
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

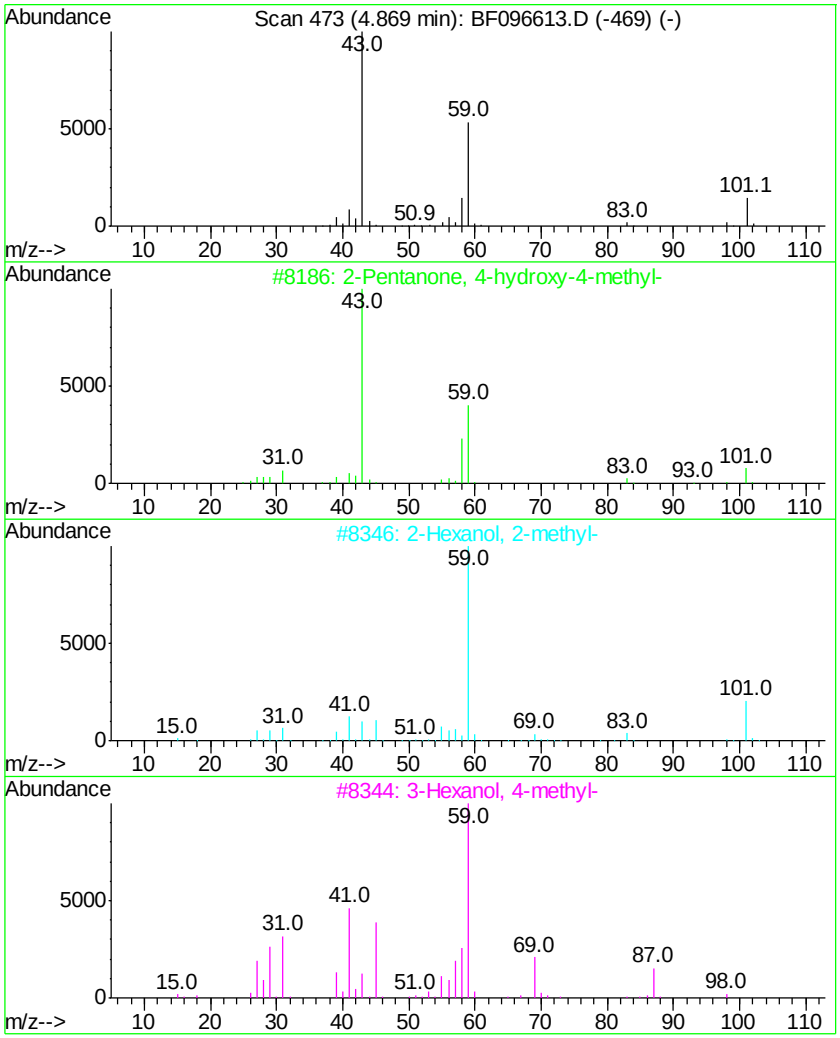
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

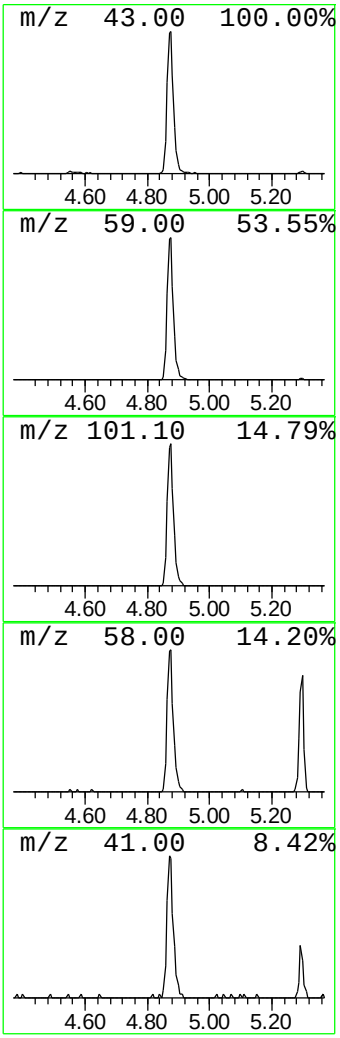
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	15.31 ng	508173	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

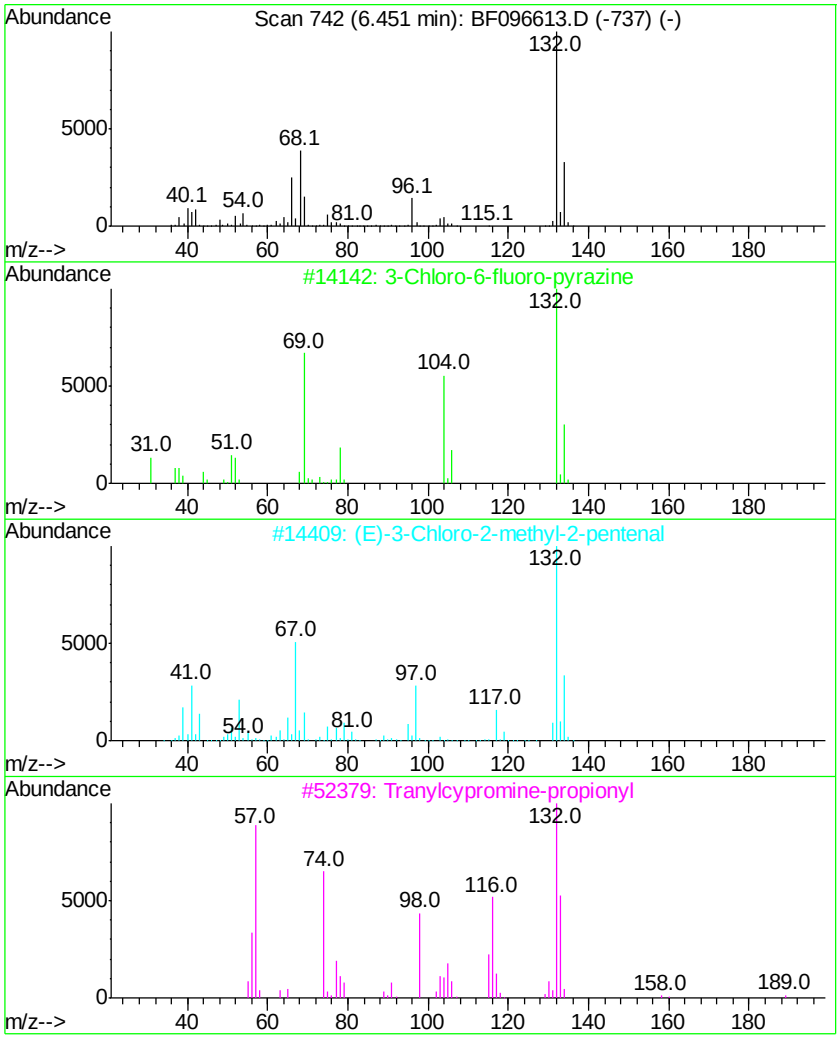
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

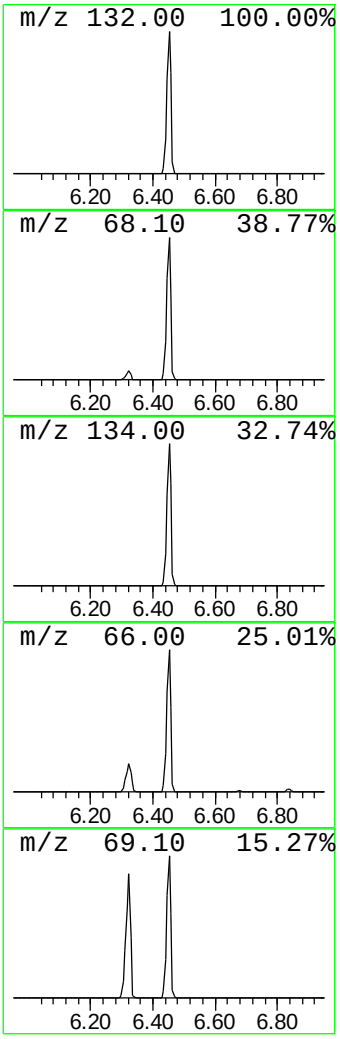
****

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	73.34 ng	2434060	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

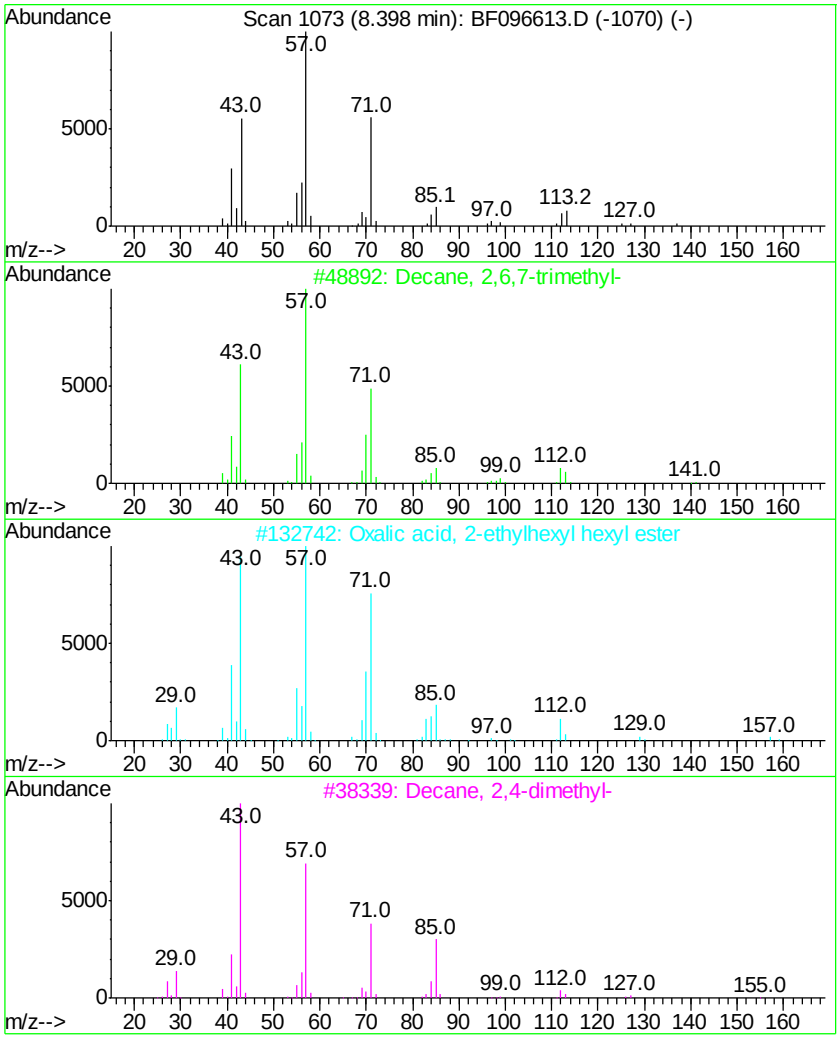
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

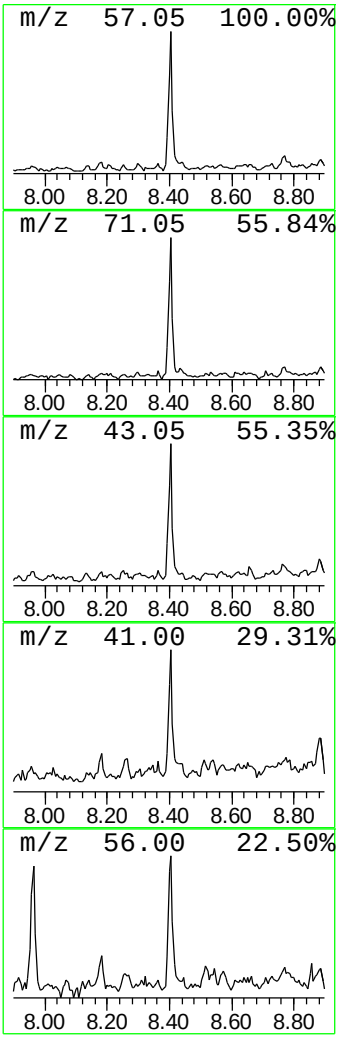
****

Peak Number 4 Decane, 2,6,7-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.40	3.00 ng	137932	Naphthalene-d8	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	64
2	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	64
3	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	59
4	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	53
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

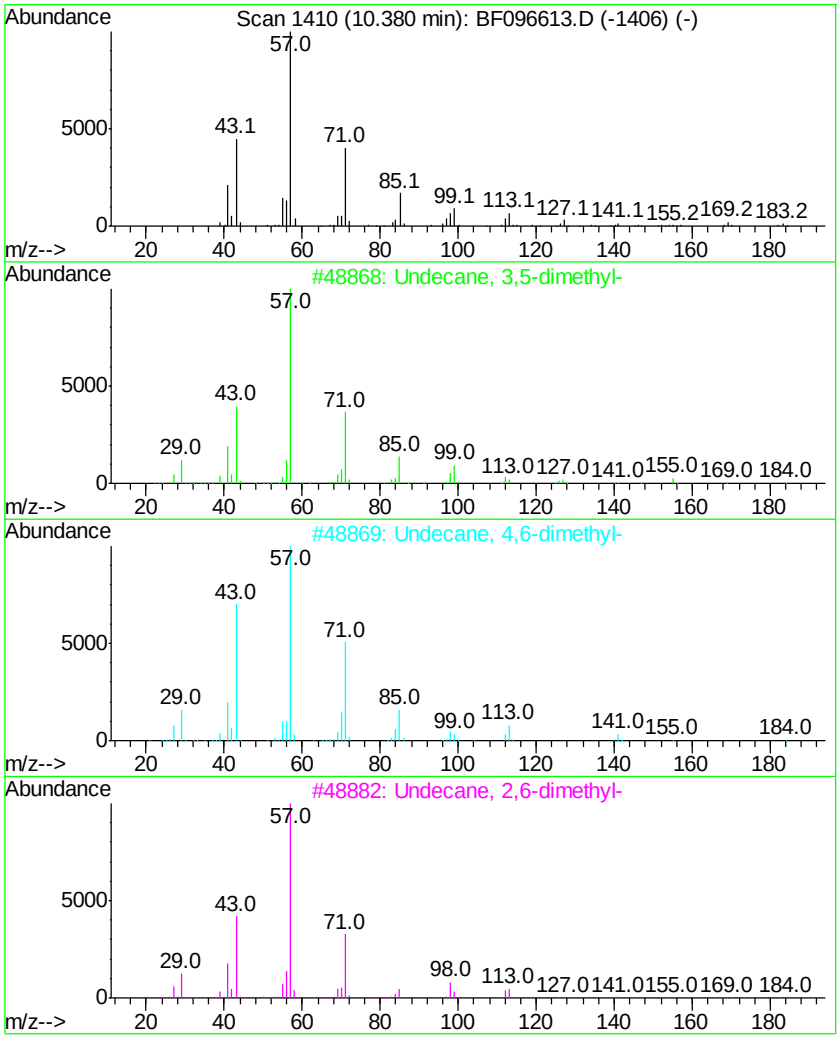
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

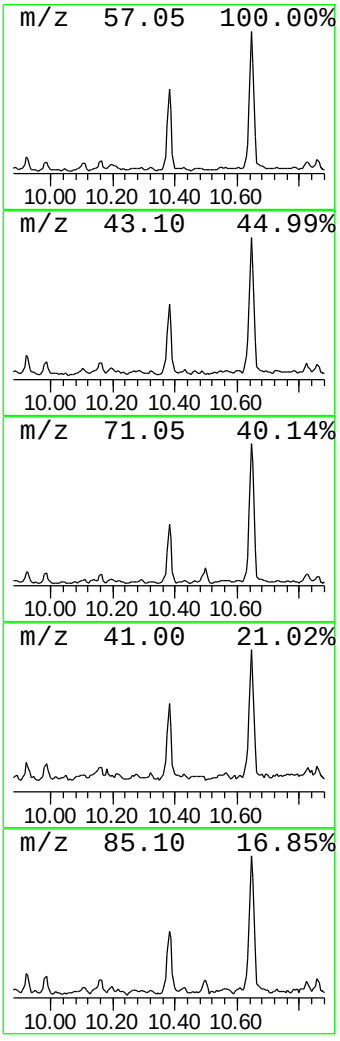
****

Peak Number 5 Undecane, 3,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	6.02 ng	306183	Acenaphthene-d10	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	90
2	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	87
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	81
4	Tetracosane	338	C24H50	000646-31-1	59
5	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

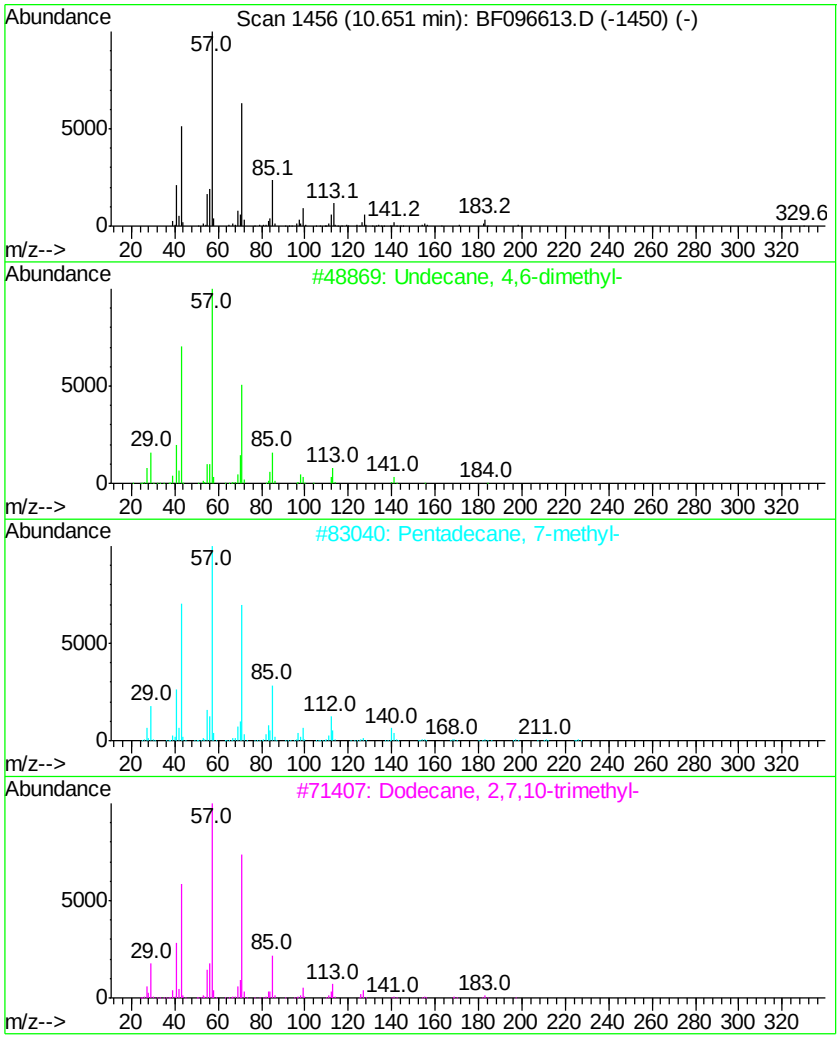
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

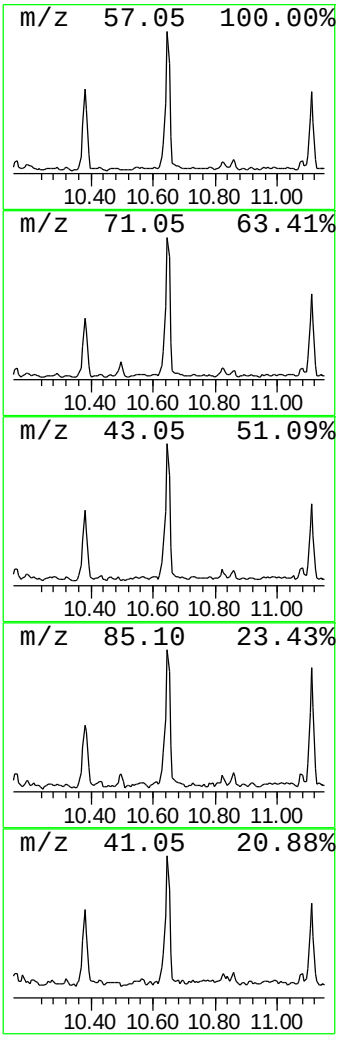
****

Peak Number 6 Undecane, 4,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	13.54 ng	642620	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	86
2	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	78
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
4	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	53
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

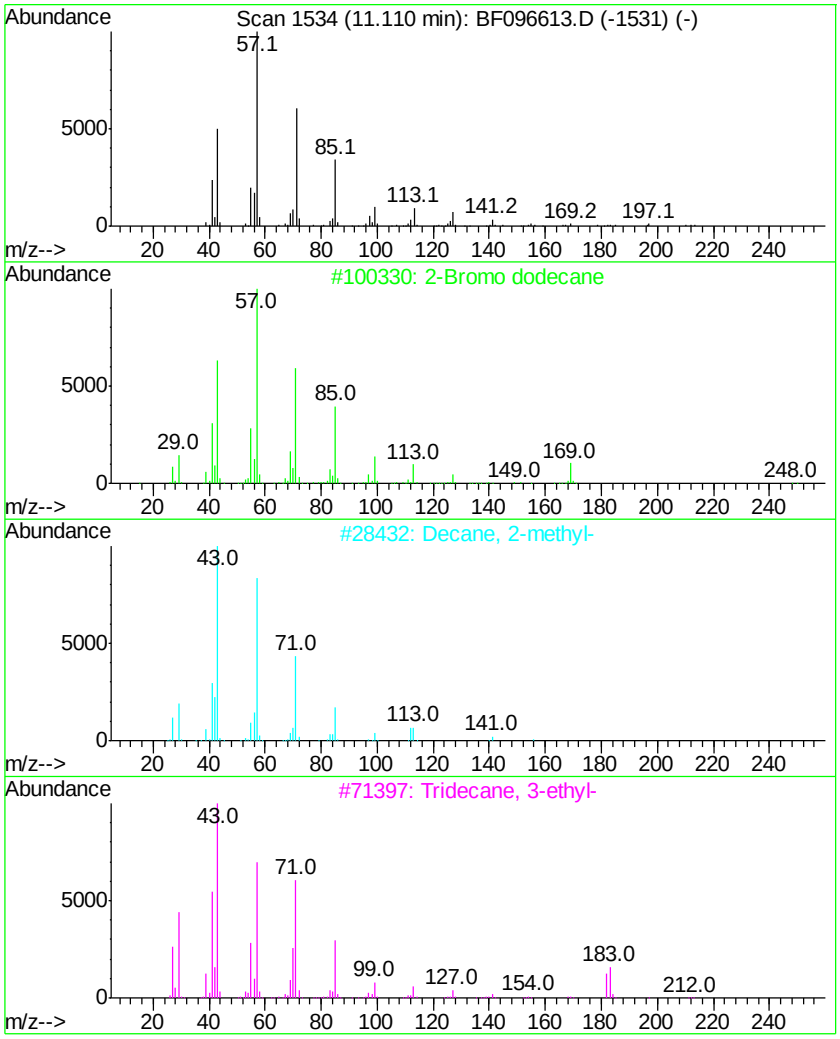
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

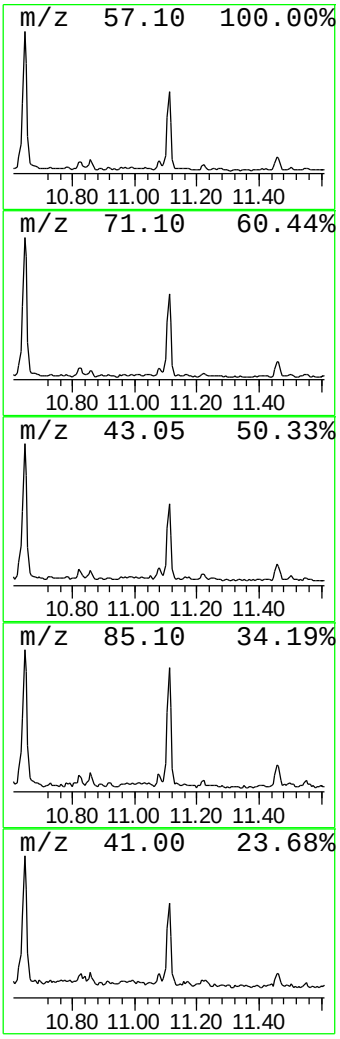
****

Peak Number 7 2-Bromo dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.11	7.43 ng	352580	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
2	Decane, 2-methyl-	156	C11H24	006975-98-0	87
3	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	86
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
5	Heptacosane	380	C27H56	000593-49-7	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

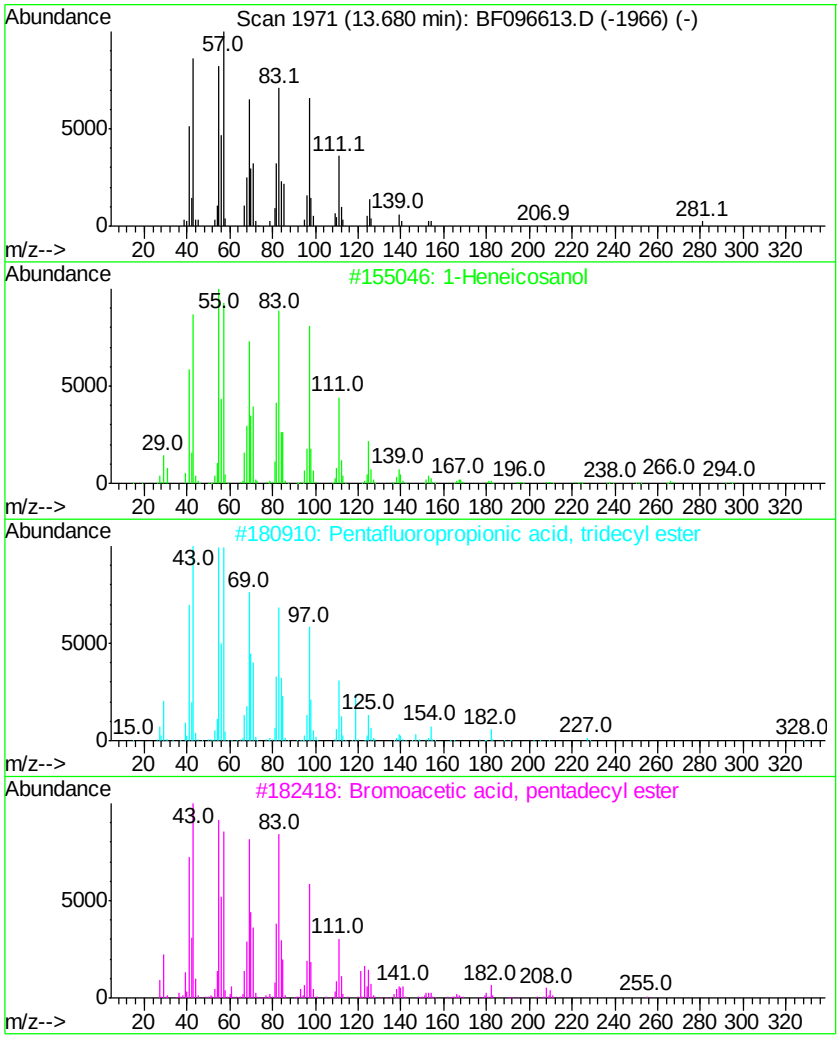
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

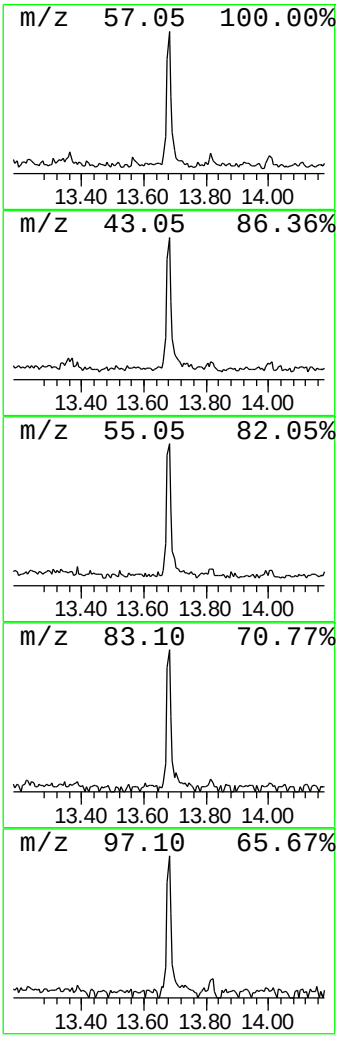
****

Peak Number 8 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	3.57 ng	136640	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	91
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

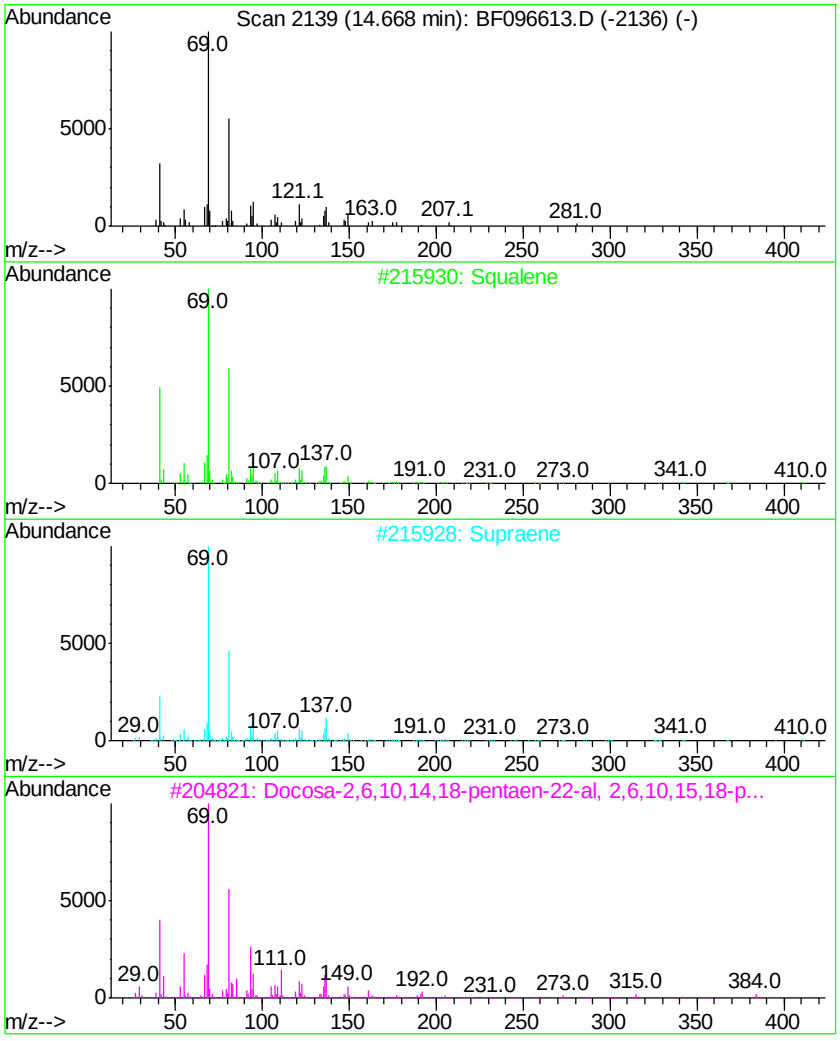
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

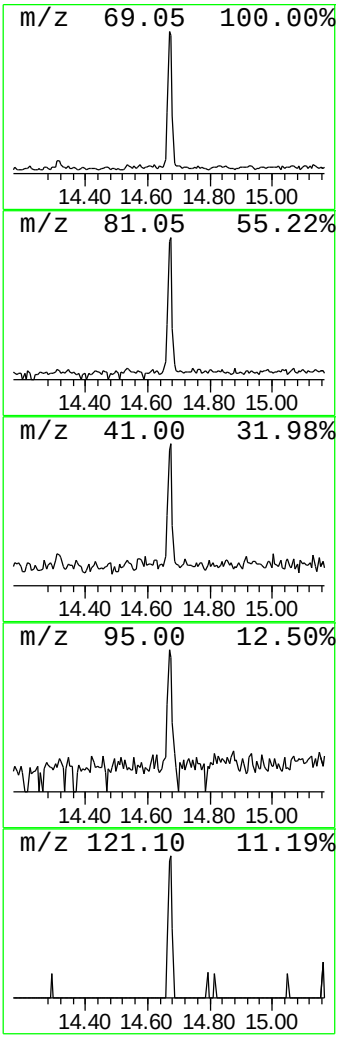
****

Peak Number 9 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.20 ng	61740	Perylene-d12	15.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
5	trans-Farnesol	222	C15H26O	000106-28-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071017\
Data File : BF096613.D
Acq On : 10 Jul 2017 20:53
Operator : SJ/JU
Sample : I4084-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP9-MH2108-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	15.3	ng	508173	1	6.68	663810	20.0
unknown6.45	6.45	73.3	ng	2434060	1	6.68	663810	20.0
Decane, 2,6,7-tri...	8.40	3.0	ng	137932	2	7.96	919922	20.0
Undecane, 3,5-dim...	10.38	6.0	ng	306183	3	9.71	1017100	20.0
Undecane, 4,6-dim...	10.65	13.5	ng	642620	4	11.19	948900	20.0
2-Bromo dodecane	11.11	7.4	ng	352580	4	11.19	948900	20.0
1-Heneicosanol	13.68	3.6	ng	136640	5	13.82	765598	20.0
Squalene	14.67	2.2	ng	61740	6	15.22	561223	20.0