LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088909.D
Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-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-BF063016.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	1.678	6	8	14	rVV	133985	203471	9.21%	0.942%
2	1.758	14	15	17	rVV	34679	45054	2.04%	0.209%
3	1.793	17	18	28	rVV	842941	1520942	68.86%	7.039%
4	1.930	28	30	47	rVB2	43080	150518	6.81%	0.697%
5	2.890	113	114	122	rBV	14490	23572	1.07%	0.109%
6	3.256	143	146	152	rVB	12887	23096	1.05%	0.107%
7	4.170	223	226	230	rBV	46824	73259	3.32%	0.339%
8	4.879	285	288	293	rBB	133480	201573	9.13%	0.933%
9	5.313	323	326	328	rBV	1899002	2088389	94.55%	9.665%
10	6.364	414	418	420	rBV	1494461	2208673	100.00%	10.222%
11	6.479	425	428	431	rBV	1779308	1941871	87.92%	8.987%
12	6.707	446	448	450	rBB	400230	395615	17.91%	1.831%
13	6.867	459	462	465	rBB	1676848	1473984	66.74%	6.822%
14	7.279	495	498	500	rBV	1283695	1263767	57.22%	5.849%
15	7.999	558	561	563	rBV	537407	533087	24.14%	2.467%
16	9.073	652	655	657	rBV	2124028	1905298	86.26%	8.818%
17	9.473	687	690	692	rVB	285179	335185	15.18%	1.551%
18	9.748	711	714	716	rBV	485557	503362	22.79%	2.330%
19	10.525	780	782	785	rBV2	969710	1132180	51.26%	5.240%
20	10.662	791	794	799	rBV	26810	33983	1.54%	0.157%
21	11.108	831	833	835	rBV	24949	25445	1.15%	0.118%
22	11.222	841	843	844	rBV	451262	473687	21.45%	2.192%
23	11.291	846	849	851	rVB	50051	44353	2.01%	0.205%
24	11.713	885	886	888	rBV	15618	22304	1.01%	0.103%
25	11.748	888	889	892	rVV	36633	34812	1.58%	0.161%
26	11.828	894	896	900	rBV2	53561	64667	2.93%	0.299%
27	12.011	910	912	916	rVB2	17593	25704	1.16%	0.119%
28	12.422	946	948	950	rBV	332298	278443	12.61%	1.289%
29	12.651	965	968	969	rBV	256189	305701	13.84%	1.415%
30	12.685	969	971	977	rVV	399346	563656	25.52%	2.609%
31	12.799	979	981	984	rVV	1094984	1425164	64.53%	6.596%
32	12.868	984	987	991	rVB2	16318	33816	1.53%	0.157%
33	12.982	991	997	998	rBV	42245	77460	3.51%	0.358%
34	13.051	1001	1003	1004	rVV	23002	31715	1.44%	0.147%

LSC Area Percent Report

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Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.085	1004	1006	1008	rVV	24564	28295	1.28%	0.131%
36	13.382	1027	1032	1037	rBV3	11559	31269	1.42%	0.145%
37	13.474	1037	1040	1045	rBV2	14212	36962	1.67%	0.171%
38	13.588	1048	1050	1052	rBV2	23139	32472	1.47%	0.150%
39	13.702	1057	1060	1064	rBV3	59361	105849	4.79%	0.490%
40	13.839	1069	1072	1079	rVB2	526840	753412	34.11%	3.487%
41	13.977	1083	1084	1086	rVB	19853	23616	1.07%	0.109%
42	14.228	1102	1106	1107	rBV	29473	41531	1.88%	0.192%
43	14.342	1112	1116	1120	rVB4	20169	58200	2.64%	0.269%
44	14.697	1144	1147	1149	rBV	73432	81693	3.70%	0.378%
45	14.834	1157	1159	1164	rVB	112440	210470	9.53%	0.974%
46	14.925	1166	1167	1172	rVV	21559	37896	1.72%	0.175%
47	15.108	1180	1183	1185	rVB	48962	76593	3.47%	0.354%
48	15.154	1185	1187	1190	rVB	84247	99784	4.52%	0.462%
49	15.211	1190	1192	1195	rBV	261649	378640	17.14%	1.752%
50	15.702	1232	1235	1238	rVB4	13522	34103	1.54%	0.158%
51	16.491	1301	1304	1309	rBV2	31603	61431	2.78%	0.284%
52	16.880	1335	1338	1347	rVB	23681	51101	2.31%	0.237%

Sum of corrected areas: 21607123

LSC Report - Integrated Chromatogram

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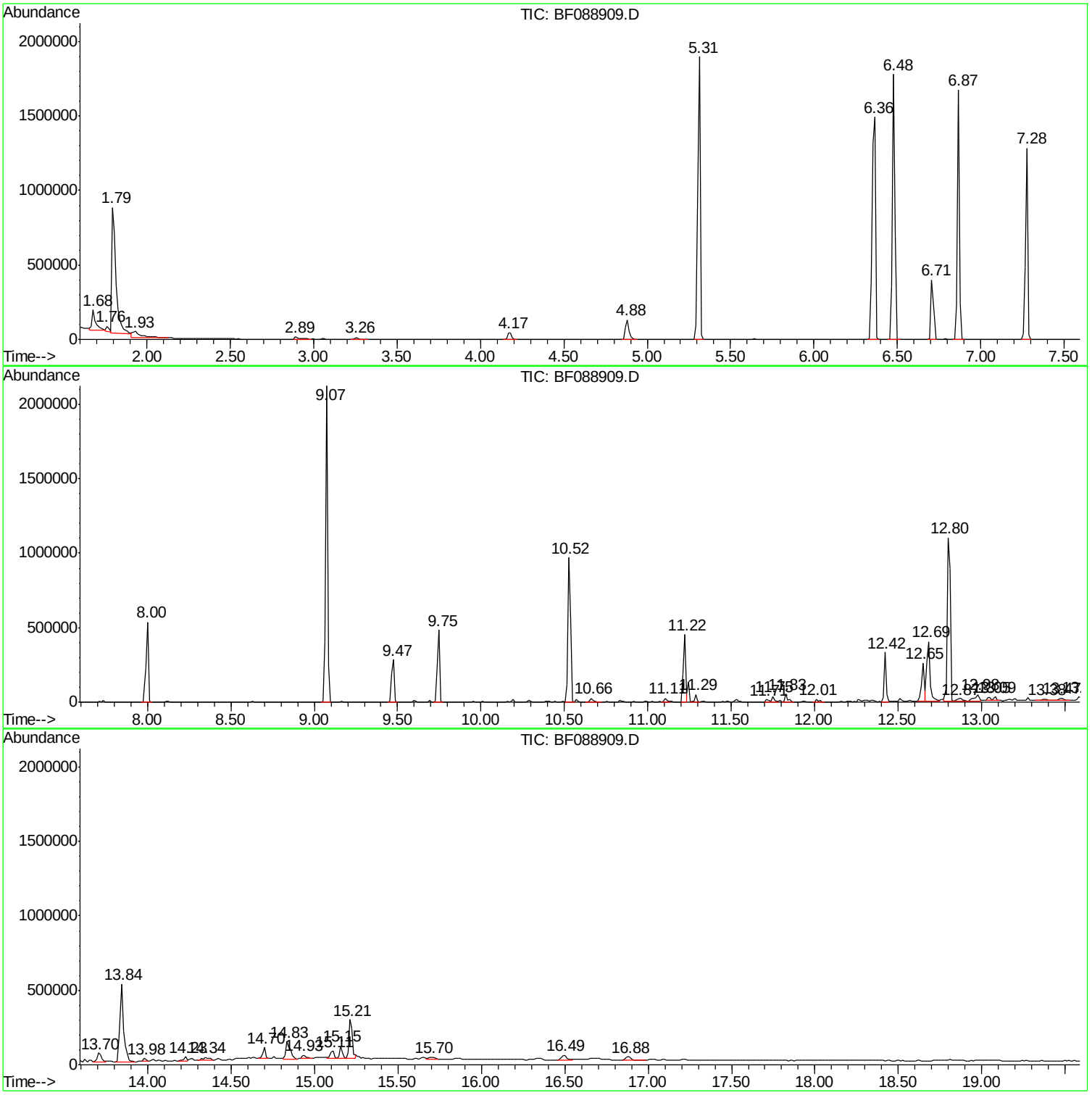
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088909.D
Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

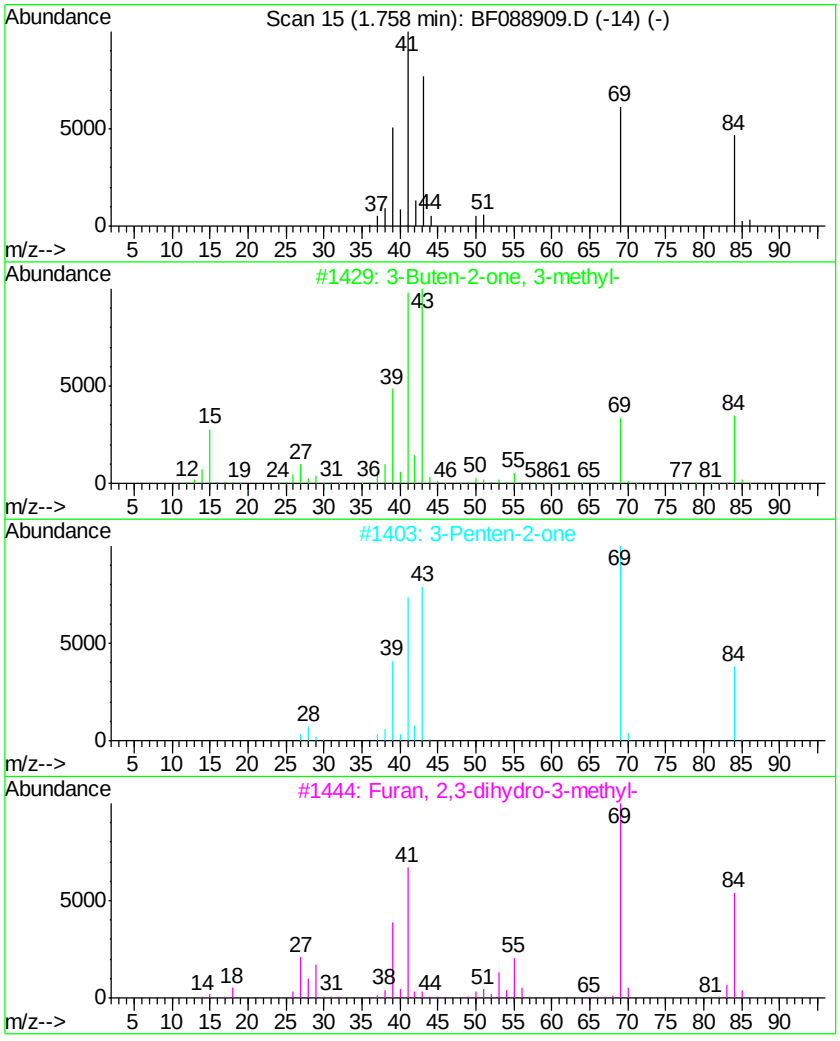
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

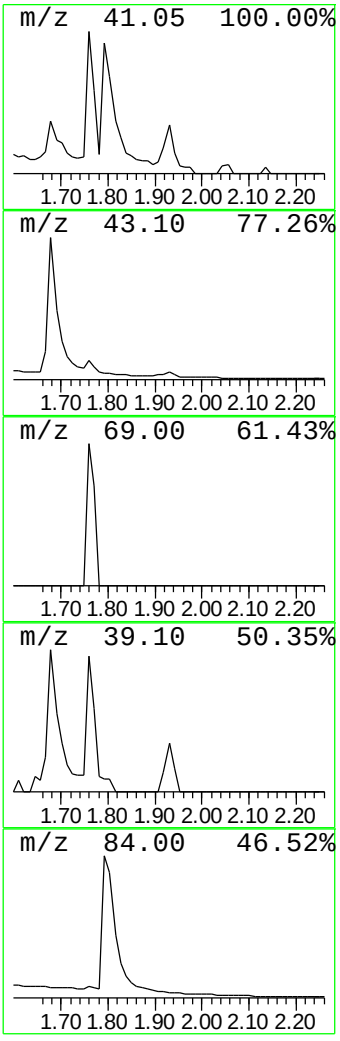
****

Peak Number 2 3-Buten-2-one, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	2.28 ng	45054	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	86
2	3-Penten-2-one	84	C5H8O	000625-33-2	72
3	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	59
4	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	52
5	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088909.D
Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

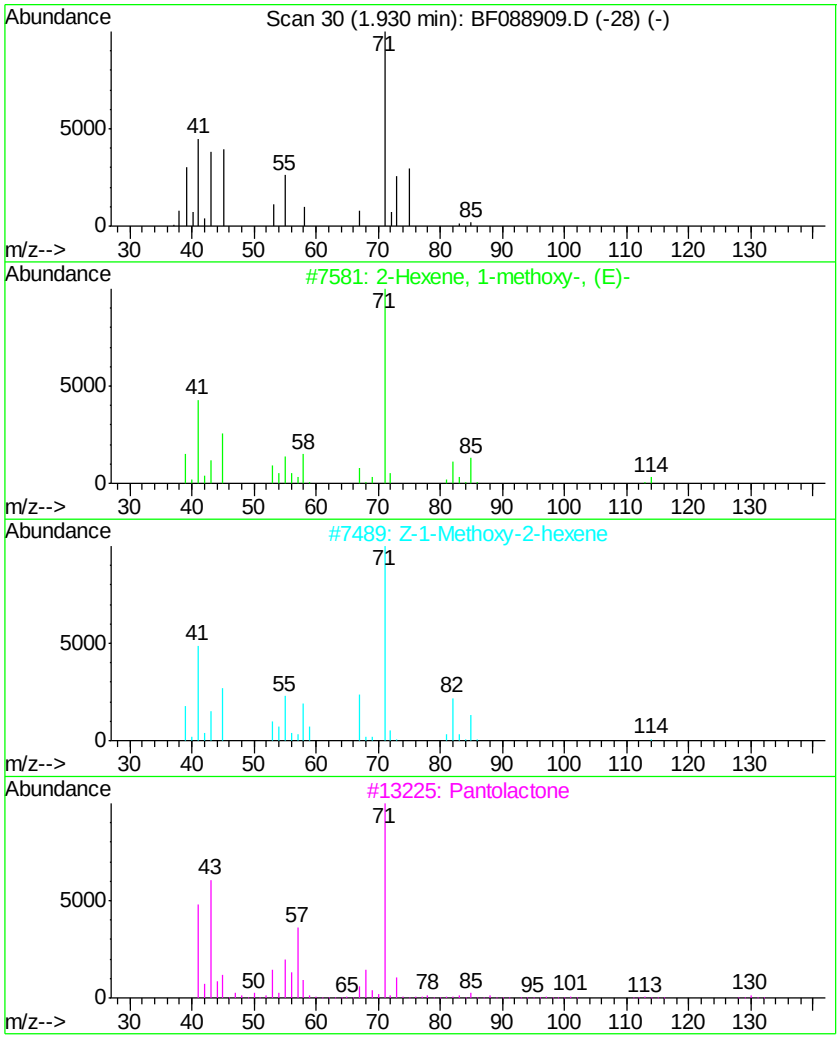
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

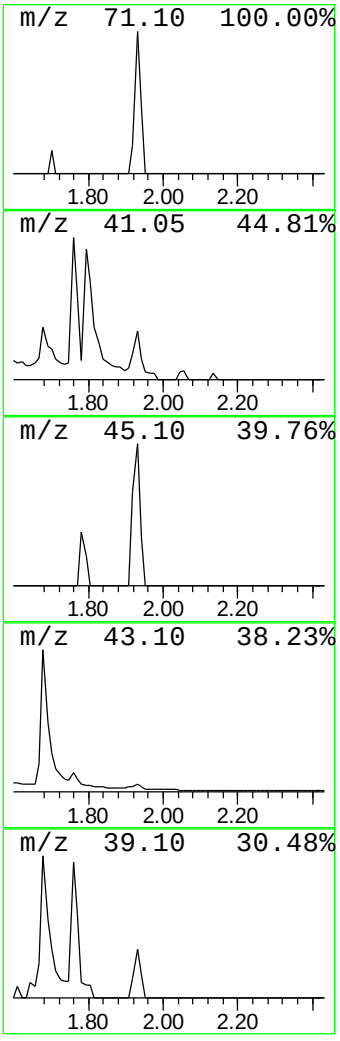
****

Peak Number 4 2-Hexene, 1-methoxy-, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.93	7.61 ng	150518	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	53
2	Z-1-Methoxy-2-hexene	114	C7H14O	1000279-60-9	42
3	Pantolactone	130	C6H10O3	000599-04-2	9
4	1,2,3-Thiadiazole, 5-methyl-	100	C3H4N2S	050406-54-7	9
5	Butanoic acid, (tetrahydro-2-fur...	172	C9H16O3	002217-33-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088909.D
Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

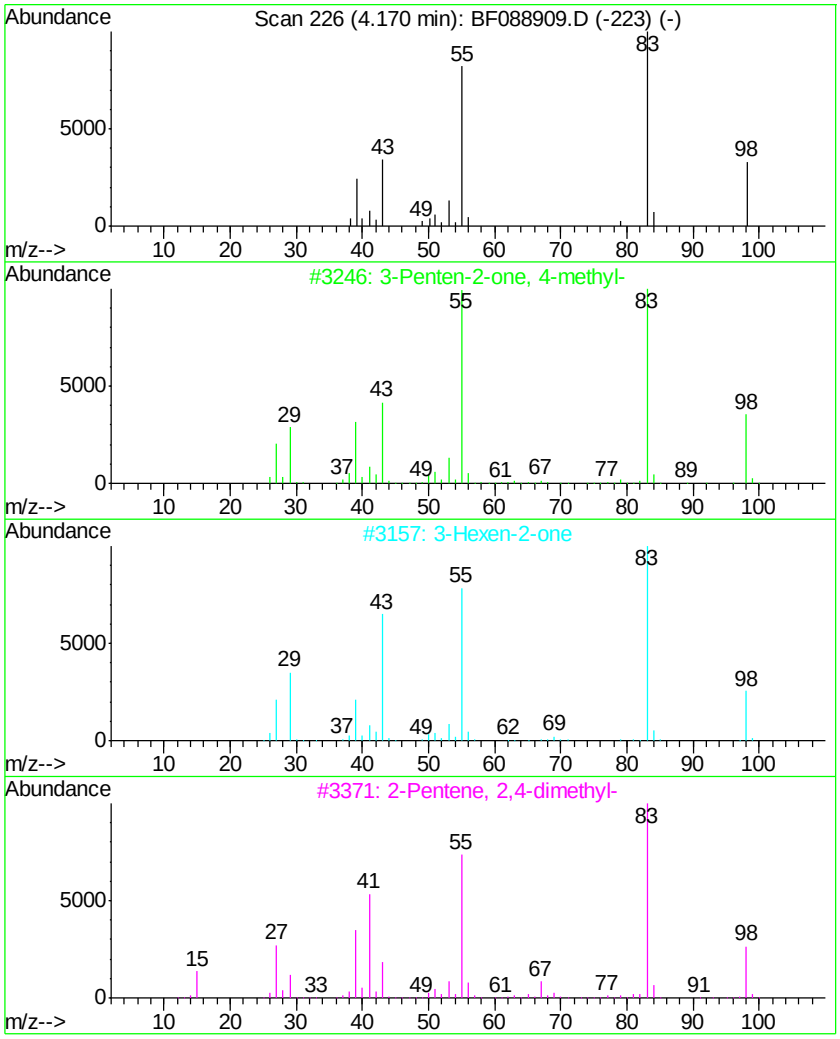
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

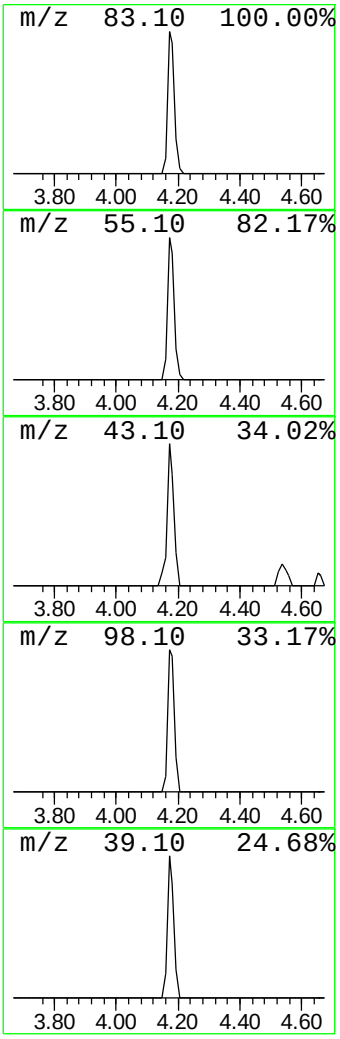
****

Peak Number 5 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.17	3.70 ng	73259	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72





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Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

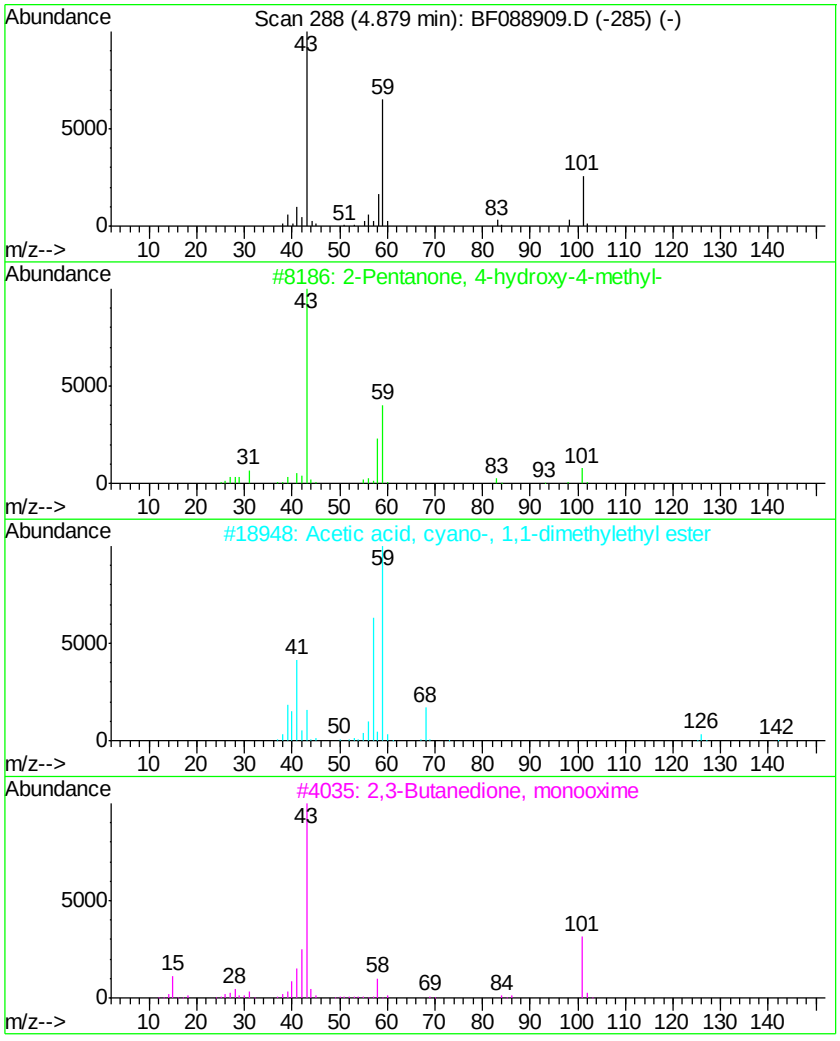
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

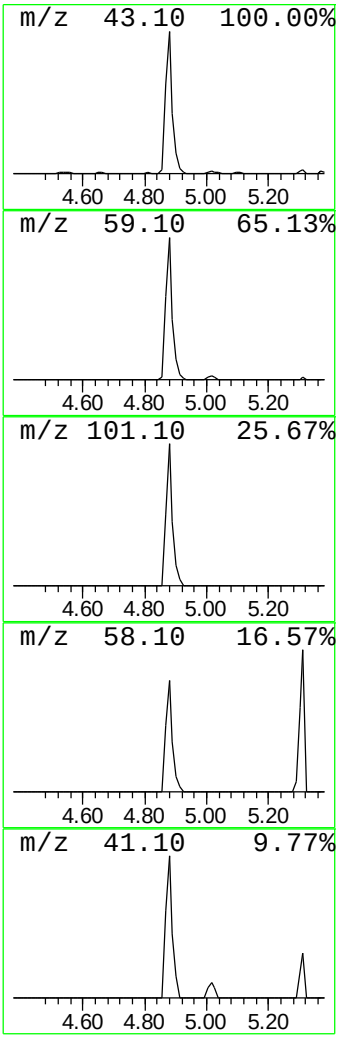
****

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	10.19 ng	201573	1,4-Dichlorobenzene-d4	6.71

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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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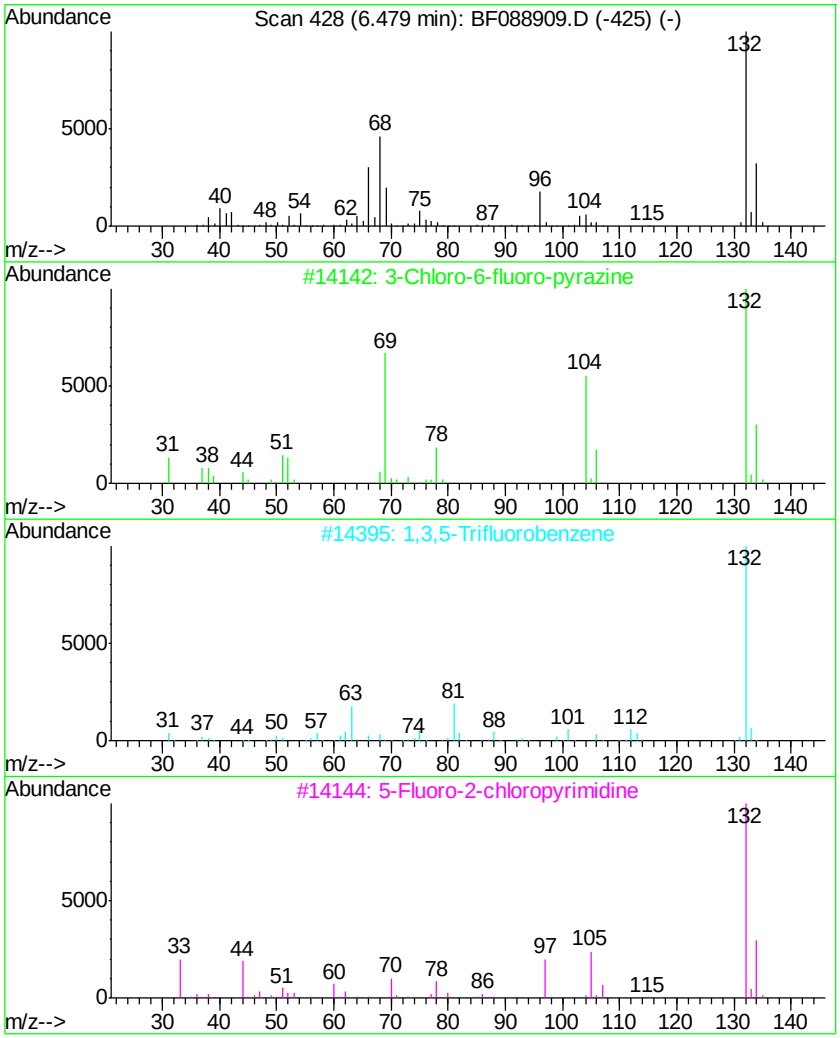
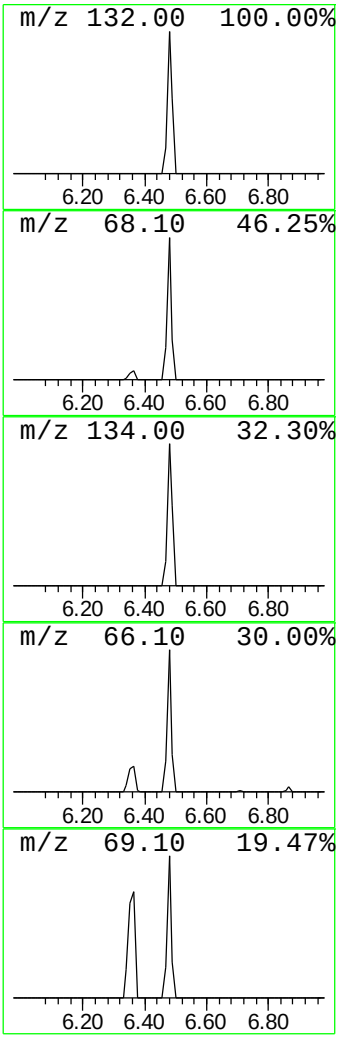
****

Peak Number 7 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	98.17 ng	1941870	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088909.D
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

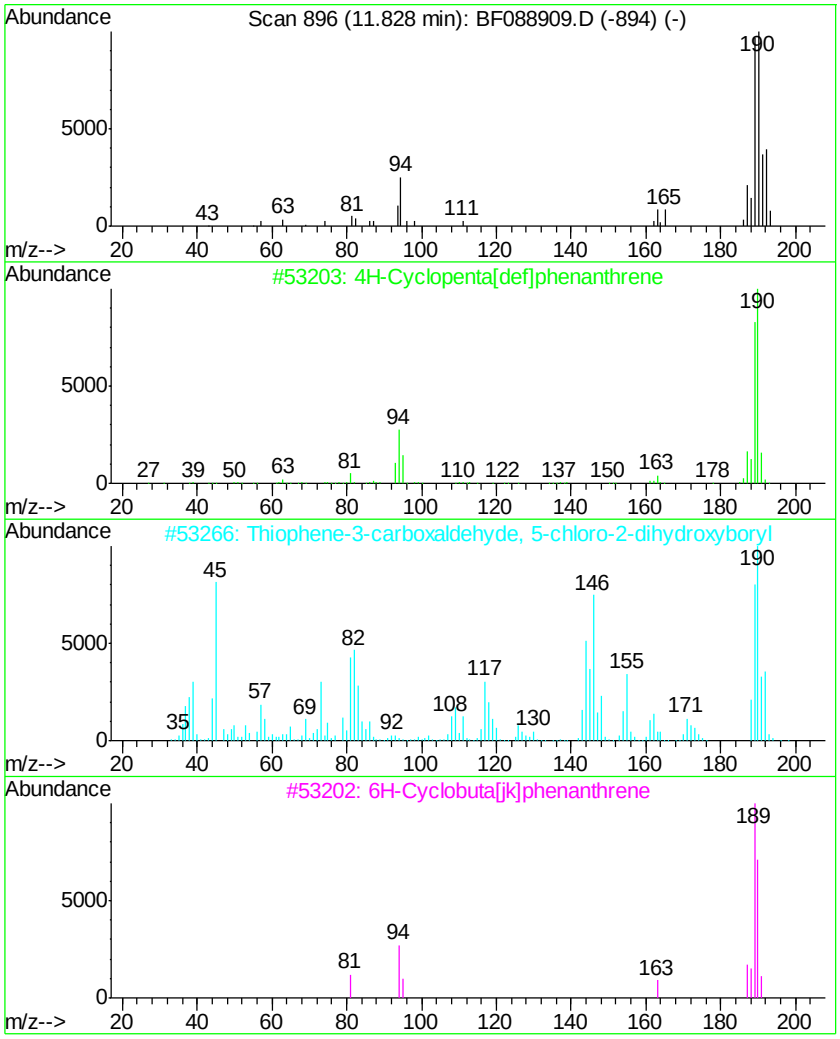
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

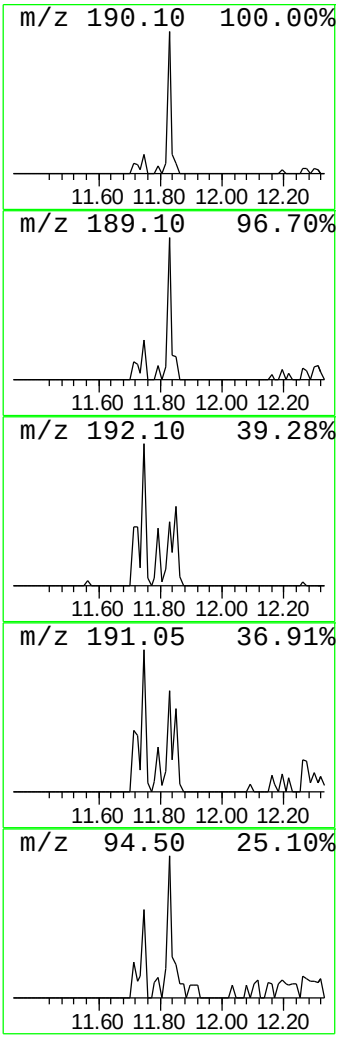
****

Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	2.73 ng	64667	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	45
4	Methyl diselenide	190	C2H6Se2	007101-31-7	43
5	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	42





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Data File : BF088909.D
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Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

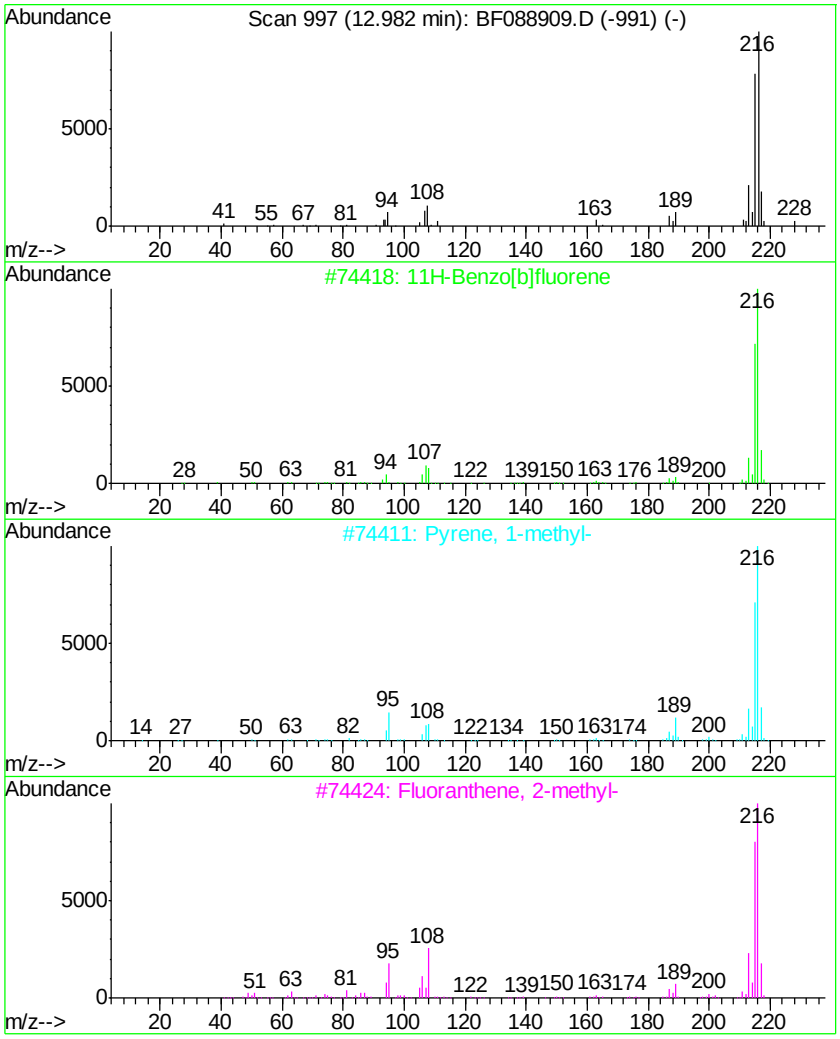
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

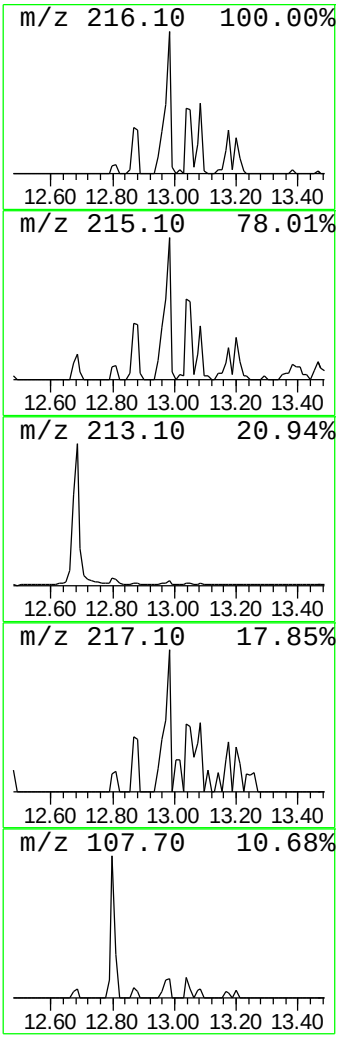
****

Peak Number 10 11H-Benzo[b]fluorene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	2.06 ng	77460	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088909.D
Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

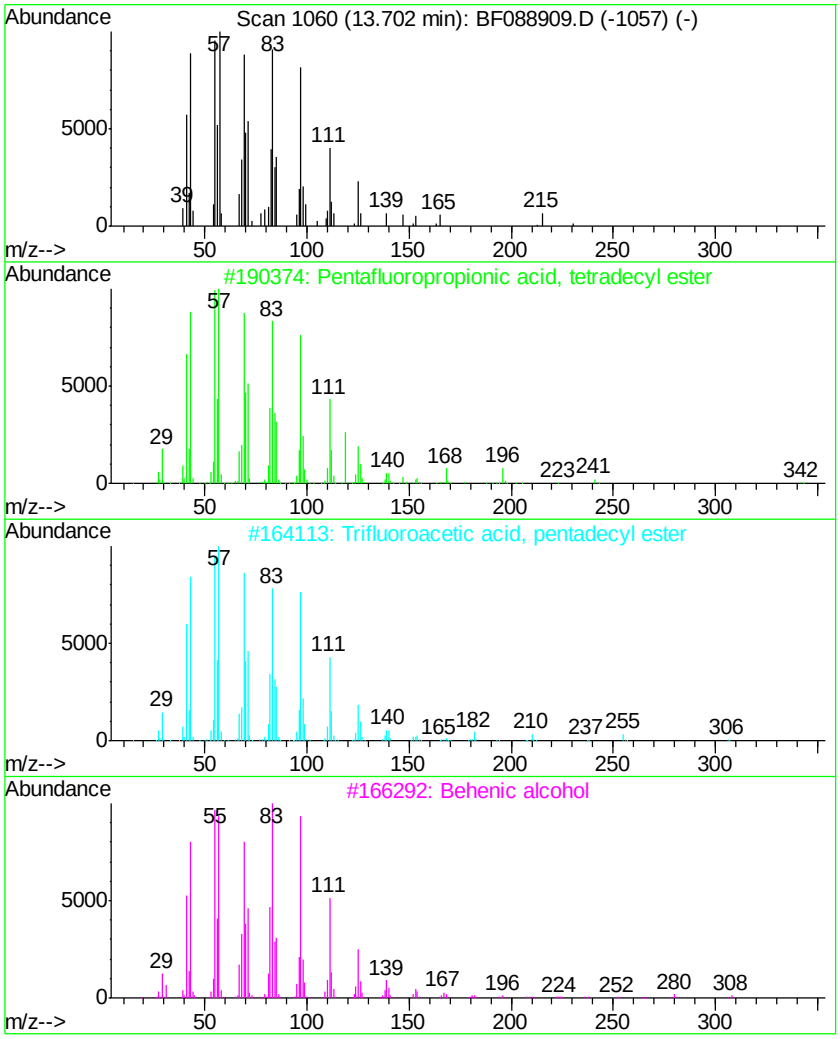
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

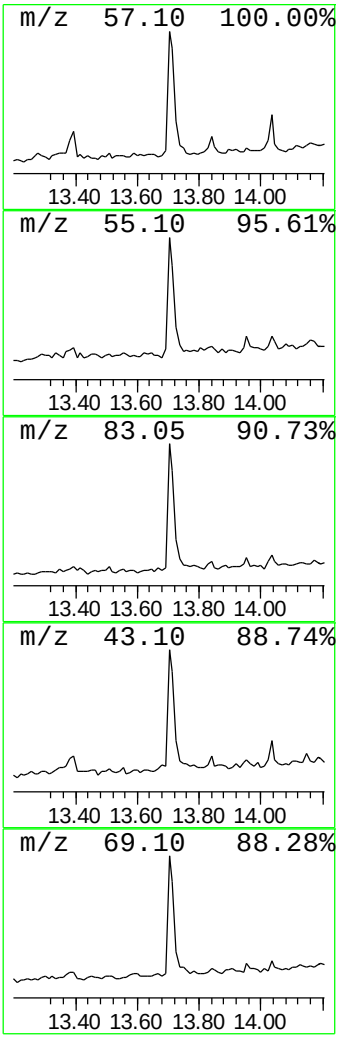
****

Peak Number 11 Pentafluoropropionic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.81 ng	105849	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088909.D
Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

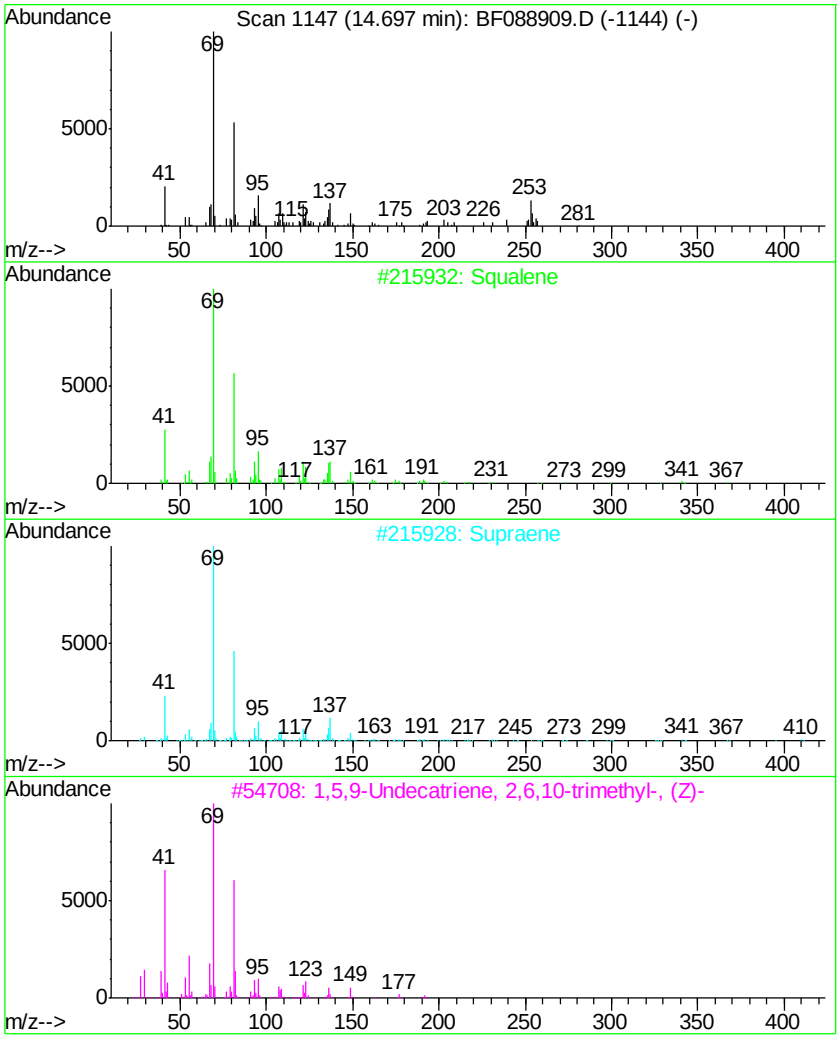
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

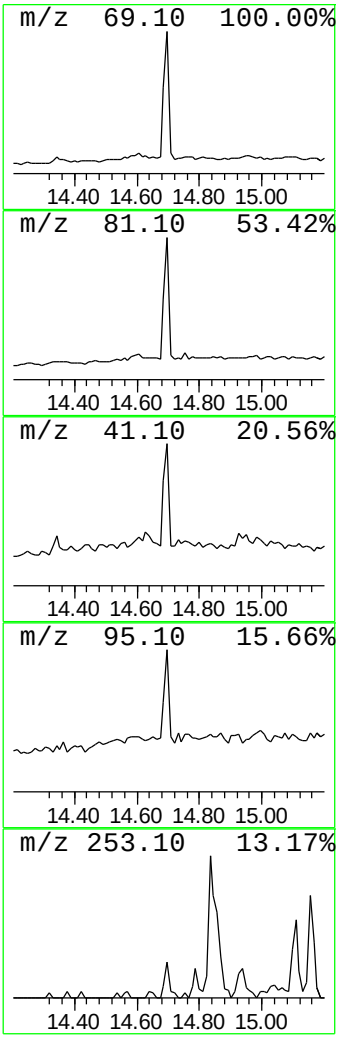
****

Peak Number 12 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	4.32 ng	81693	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	76
2	Supraene	410	C30H50	007683-64-9	68
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	62
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	50
5	trans-Farnesol	222	C15H26O	000106-28-5	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071116\
Data File : BF088909.D
Acq On : 11 Jul 2016 19:54
Operator : UM/SJ
Sample : H3915-11
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P6-B1-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
3-Buten-2-one, 3-...	1.76	2.3	ng	45054	1	6.71	395615	20.0
2-Hexene, 1-metho...	1.93	7.6	ng	150518	1	6.71	395615	20.0
3-Penten-2-one, 4...	4.17	3.7	ng	73259	1	6.71	395615	20.0
2-Pentanone, 4-hy...	4.88	10.2	ng	201573	1	6.71	395615	20.0
unknown6.48	6.48	98.2	ng	1941870	1	6.71	395615	20.0
4H-Cyclopenta[def...	11.83	2.7	ng	64667	4	11.22	473687	20.0
11H-Benzo[b]fluorene	12.98	2.1	ng	77460	5	13.84	753412	20.0
Pentafluoropropio...	13.70	2.8	ng	105849	5	13.84	753412	20.0
Squalene	14.70	4.3	ng	81693	6	15.21	378640	20.0