LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-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-BF052316.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	1.644	3	5	44	rVB	2068966	3932396	99.09%	10.771%
2	4.798	278	281	297	rBV	156891	454564	11.45%	1.245%
3	5.450	336	338	358	rBV	2308110	3776656	95.16%	10.345%
4	7.096	479	482	487	rBV	2578059	3705016	93.36%	10.149%
5	7.187	487	490	502	rVB	3000198	3968585	100.00%	10.871%
6	7.519	517	519	524	rBV	551117	686136	17.29%	1.879%
7	7.759	537	540	543	rBV	2249531	2827838	71.26%	7.746%
8	8.445	596	600	602	rBV	1489848	2470290	62.25%	6.766%
9	9.553	694	697	709	rBV	659749	810605	20.43%	2.220%
10	11.336	849	853	855	rBV	2995417	3803755	95.85%	10.419%
11	11.588	873	875	880	rVB2	33959	43411	1.09%	0.119%
12	11.691	881	884	888	rVB2	63910	126762	3.19%	0.347%
13	11.771	888	891	893	rBV	181096	243911	6.15%	0.668%
14	11.816	893	895	899	rVB2	71943	110772	2.79%	0.303%
15	12.022	911	913	916	rBV	601847	804861	20.28%	2.205%
16	12.262	932	934	936	rVB	51366	62926	1.59%	0.172%
17	12.308	936	938	941	rVB	97904	117979	2.97%	0.323%
18	12.376	941	944	949	rBV	611444	795644	20.05%	2.179%
19	13.222	1015	1018	1020	rVB	44967	63735	1.61%	0.175%
20	13.474	1037	1040	1043	rVB	162874	231825	5.84%	0.635%
21	13.679	1054	1058	1064	rBV	1376057	1993501	50.23%	5.460%
22	13.988	1082	1085	1090	rBV	72227	115053	2.90%	0.315%
23	14.719	1146	1149	1151	rBV	36619	44308	1.12%	0.121%
24	14.777	1151	1154	1157	rBV	517759	643006	16.20%	1.761%
25	17.131	1357	1360	1363	rBV	2333545	2825891	71.21%	7.741%
26	17.703	1407	1410	1412	rBV	299202	394070	9.93%	1.079%
27	17.748	1412	1414	1418	rVB2	46604	65950	1.66%	0.181%
28	18.388	1467	1470	1473	rBV	36793	61253	1.54%	0.168%
29	18.468	1475	1477	1480	rBV	485672	622433	15.68%	1.705%
30	18.537	1480	1483	1487	rVB	58733	99466	2.51%	0.272%
31	19.063	1527	1529	1532	rBV	61784	84601	2.13%	0.232%
32	19.509	1566	1568	1574	rBV2	24544	56289	1.42%	0.154%
33	19.611	1574	1577	1579	rBV	32170	44940	1.13%	0.123%
34	20.137	1621	1623	1629	rBV	268171	419242	10.56%	1.148%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-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-BF052316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

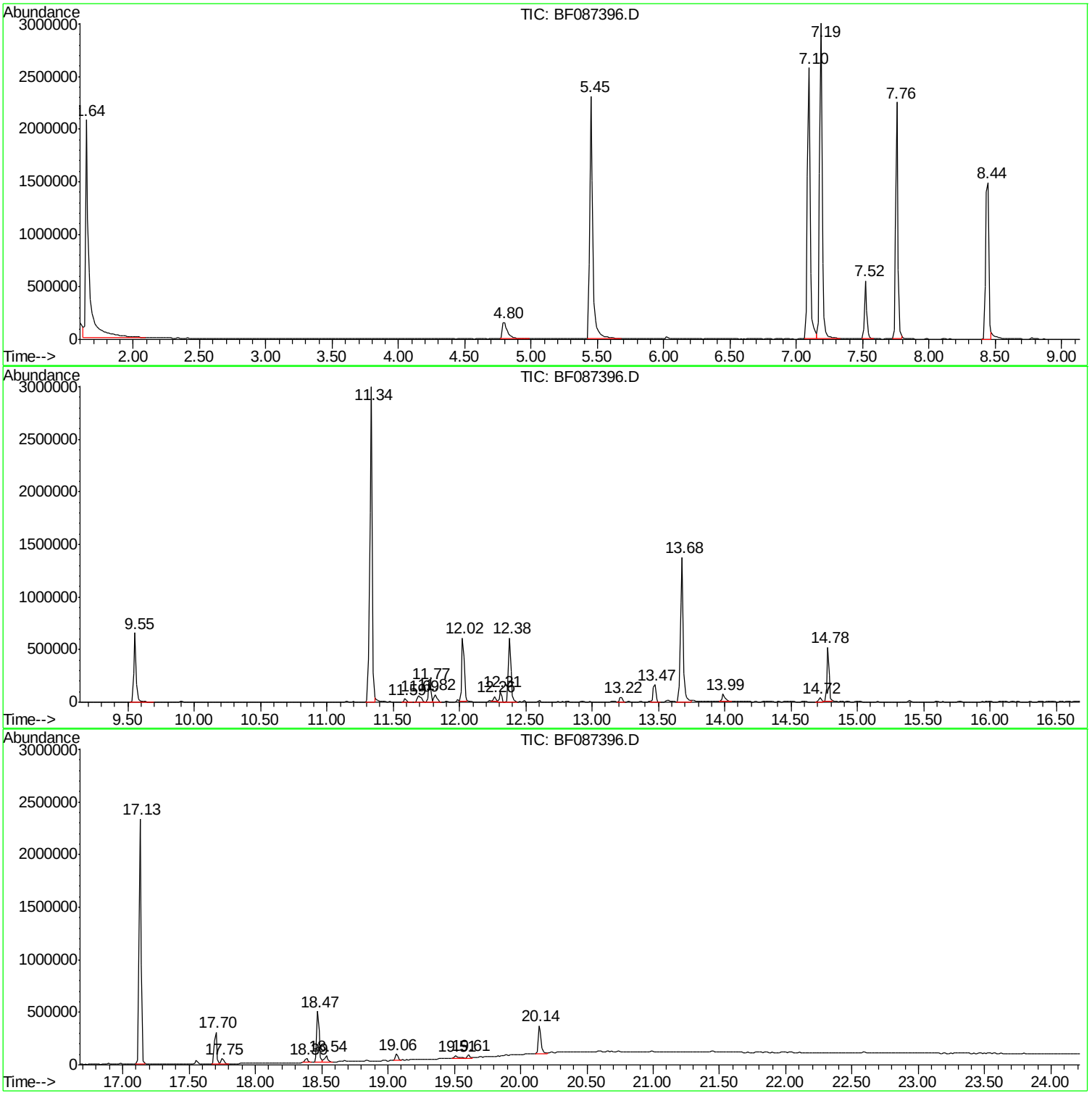
Sum of corrected areas: 36507670

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : H3220-04
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Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

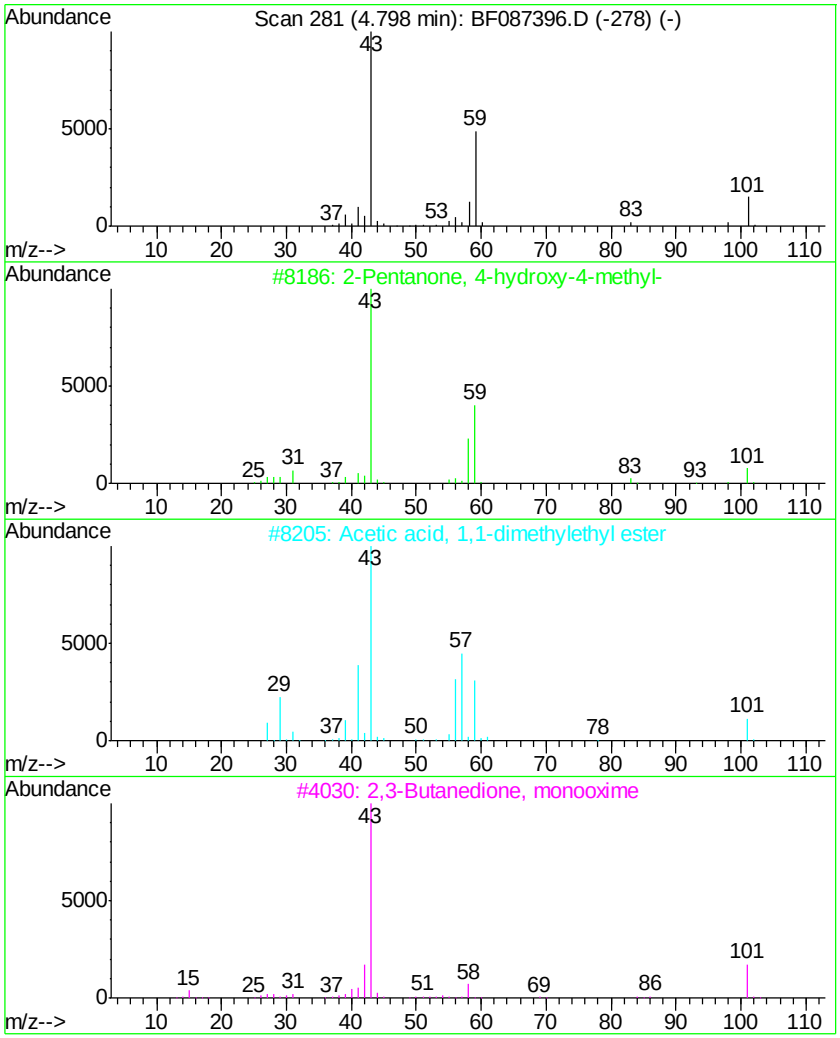
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

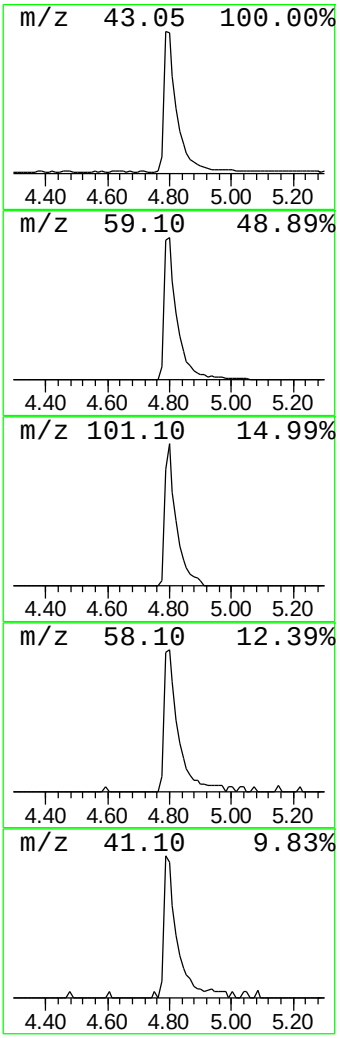
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	13.25 ng	454564	1,4-Dichlorobenzene-d4	7.52

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

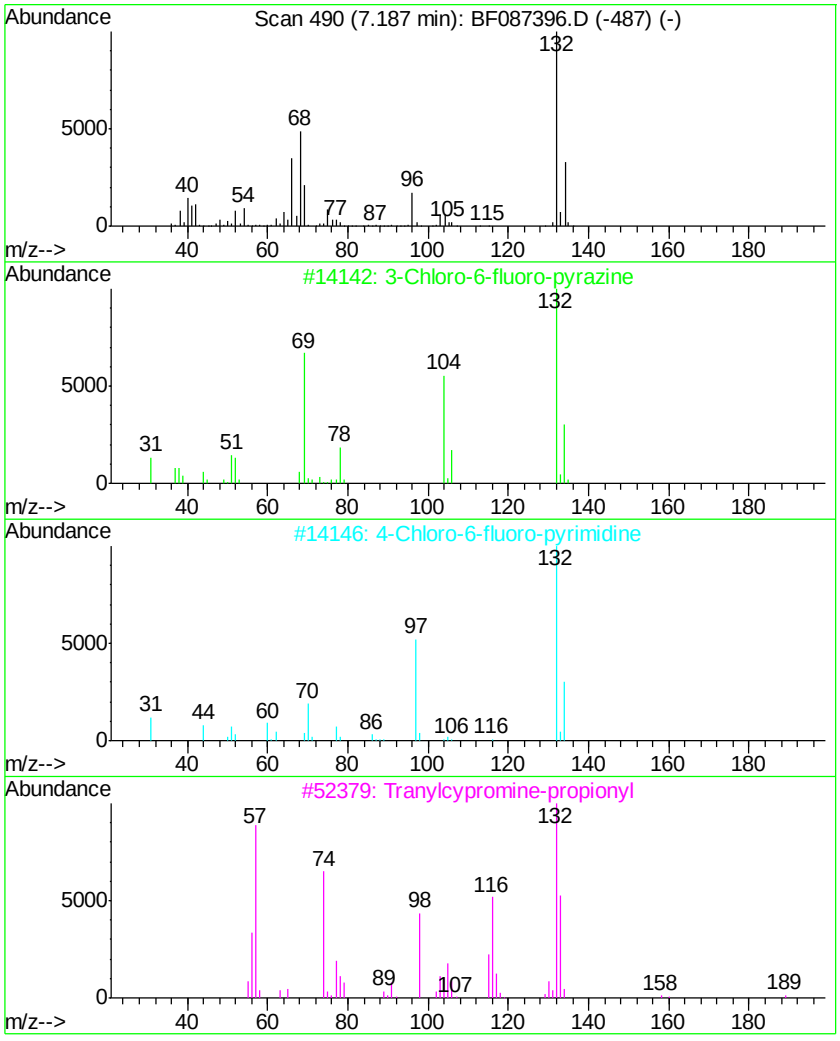
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

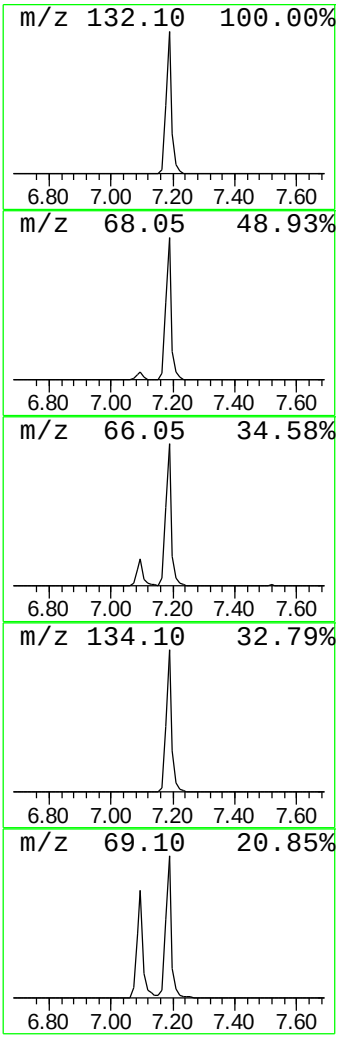
****

Peak Number 3 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	115.68 ng	3968590	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Acq On : 26 May 2016 5:20
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Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

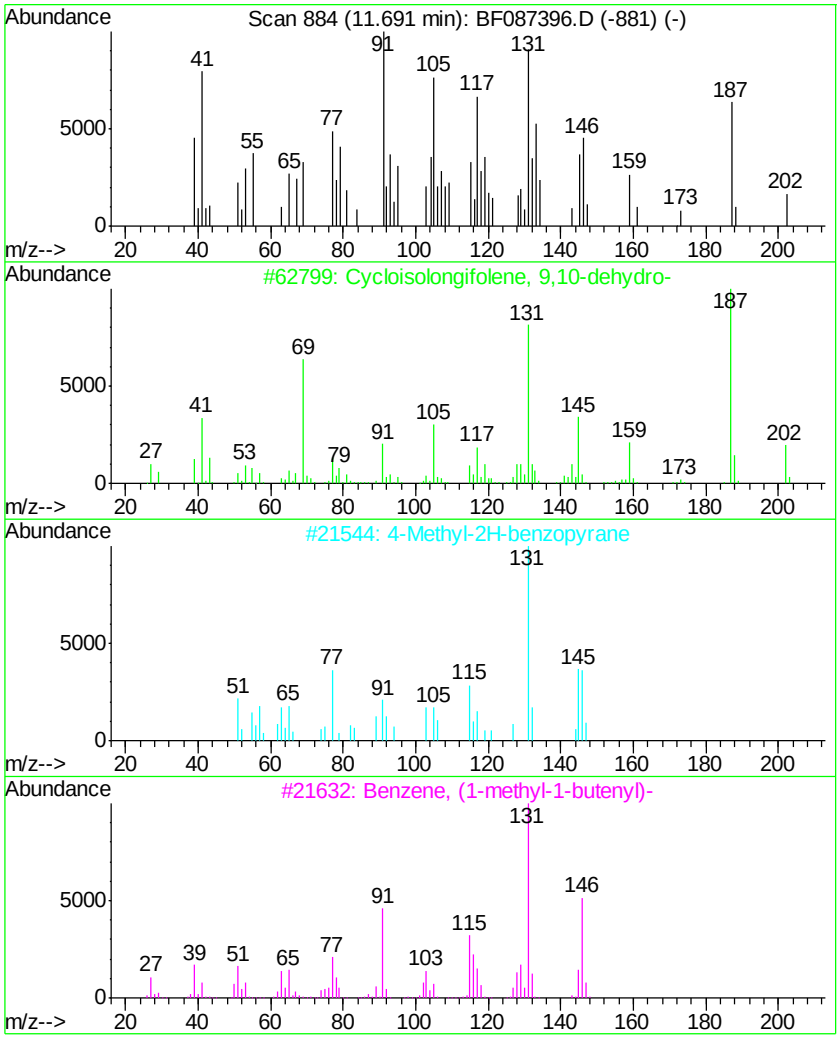
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

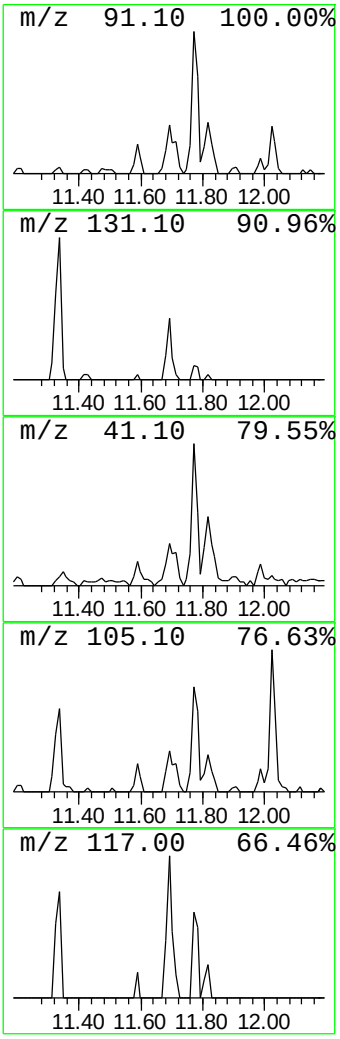
****

Peak Number 5 Cycloisolongifolene, 9,10-d... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	3.19 ng	126762	Acenaphthene-d10	12.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloisolongifolene, 9,10-dehydro-	202	C15H22	1000156-81-6	60
2	4-Methyl-2H-benzopyrane	146	C10H10O	021776-94-3	46
3	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	46
4	Biphenylene, 1,2,3,6,7,8,8a,8b-o...	188	C14H20	106988-87-8	46
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	41





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

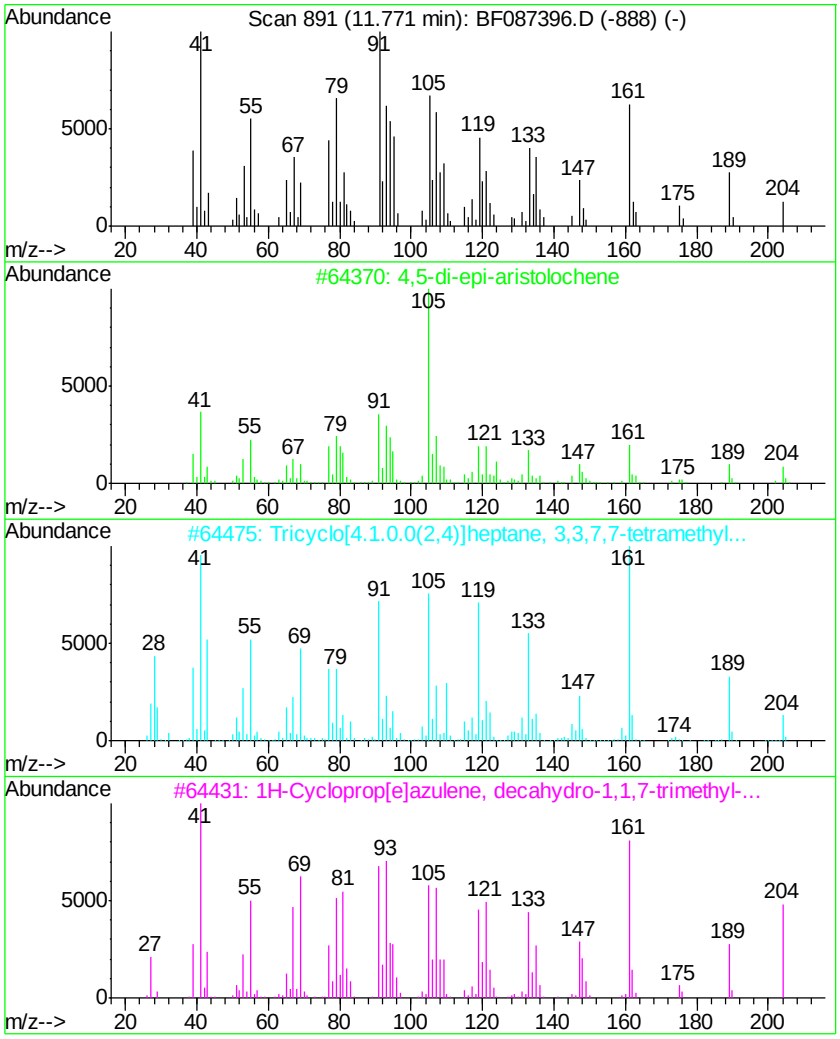
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

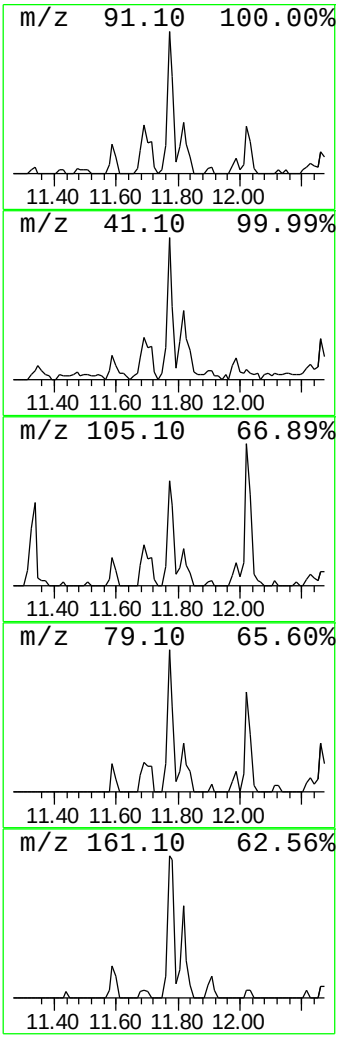
****

Peak Number 6 4,5-di-epi-aristolochene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	6.13 ng	243911	Acenaphthene-d10	12.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,5-di-epi-aristolochene	204	C15H24	1000374-17-1	80
2	Tricyclo[4.1.0.0(2,4)]heptane, 3...	204	C15H24	056348-21-1	70
3	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	68
4	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	64
5	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	55





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

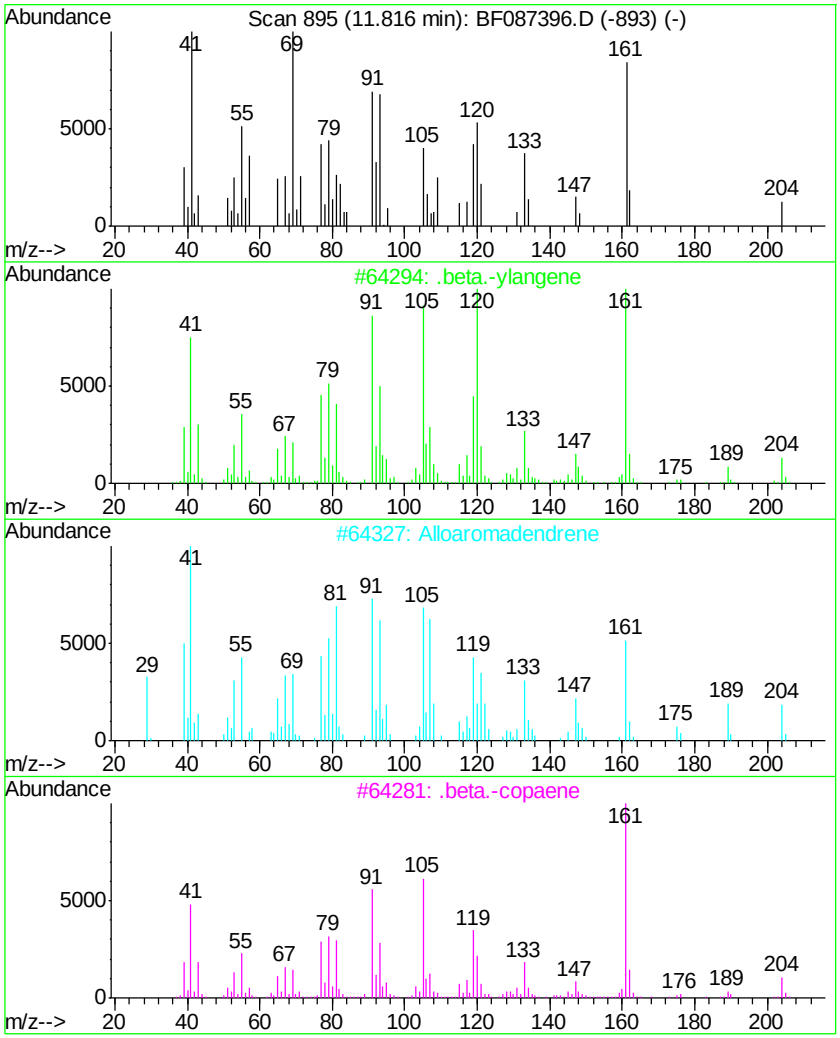
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

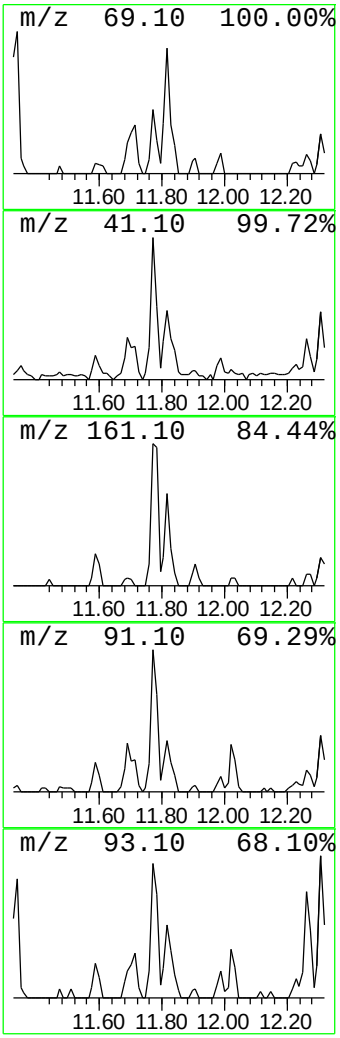
****

Peak Number 7 .beta.-ylangene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.78 ng	110772	Acenaphthene-d10	12.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-ylangene	204	C15H24	1000374-19-1	78
2	Alloaromadendrene	204	C15H24	025246-27-9	50
3	.beta.-copaene	204	C15H24	1000374-18-9	46
4	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	46
5	Cyclohexene, 3-(1,5-dimethyl-4-h...	204	C15H24	020307-83-9	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

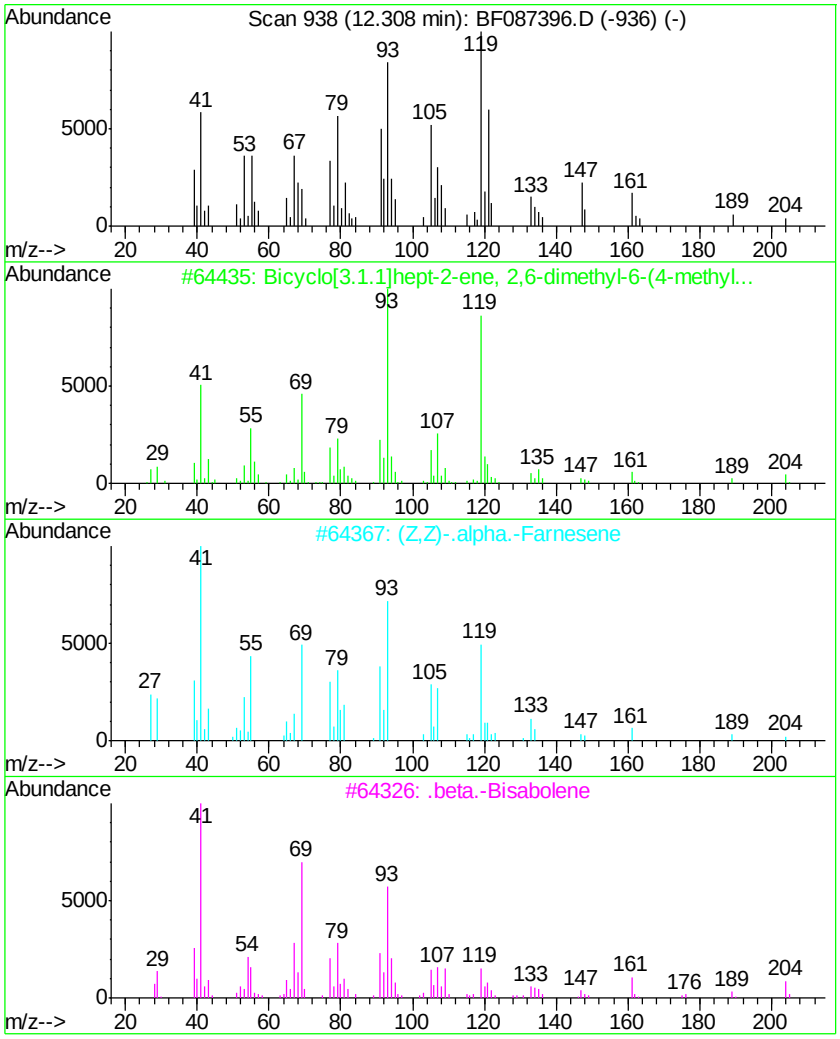
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

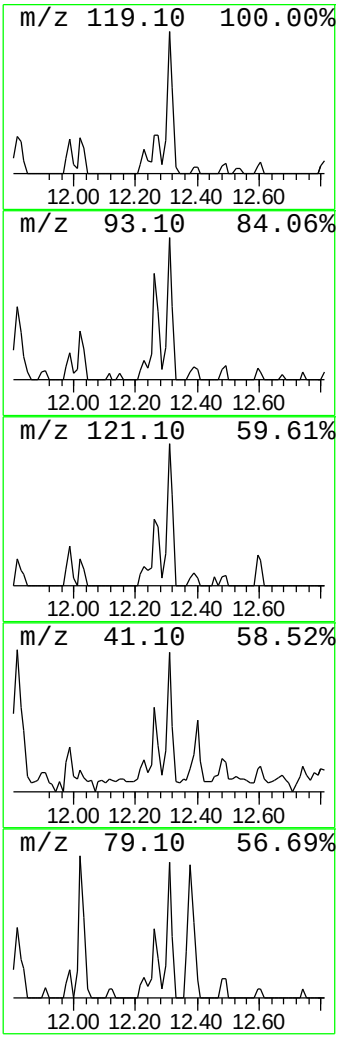
****

Peak Number 8 Bicyclo[3.1.1]hept-2-ene, 2... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	2.97 ng	117979	Acenaphthene-d10	12.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]hept-2-ene, 2,6-di...	204	C15H24	017699-05-7	58
2	(Z,Z)-.alpha.-Farnesene	204	C15H24	1000293-03-1	58
3	.beta.-Bisabolene	204	C15H24	000495-61-4	55
4	Bicyclo[3.1.1]heptane, 6-methyl-...	204	C15H24	055123-21-2	53
5	1-Methylene-2-vinylcyclopentane	108	C8H12	006196-78-7	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
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Sample : H3220-04
Misc :
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Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

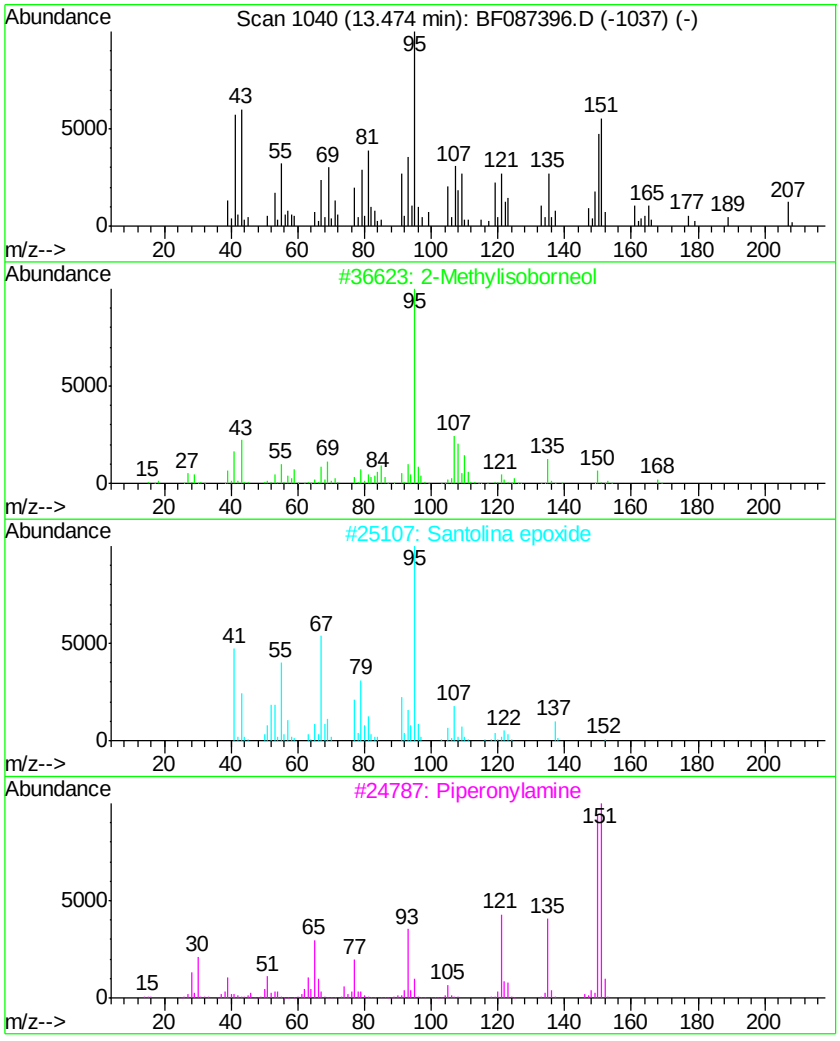
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

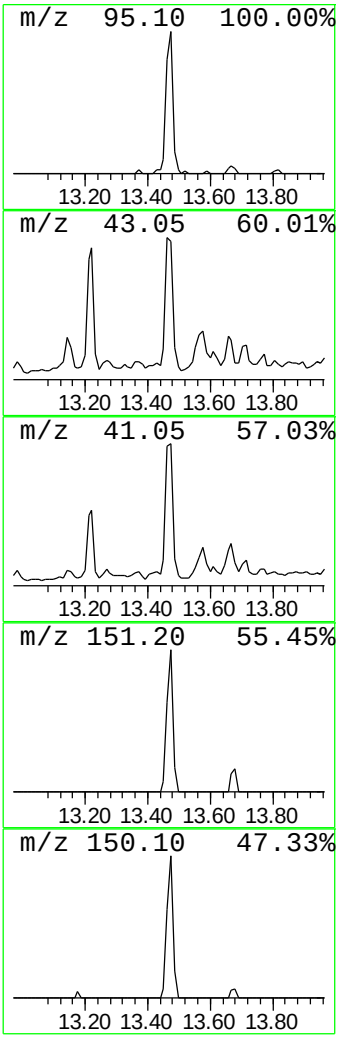
****

Peak Number 9 unknown13.47 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	5.83 ng	231825	Acenaphthene-d10	12.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylisoborneol	168	C11H20O	002371-42-8	38
2	Santolina epoxide	152	C10H16O	060485-45-2	27
3	Piperonylamine	151	C8H9NO2	002620-50-0	25
4	2-Furoic acid, but-3-yn-2-yl ester	164	C9H8O3	1000299-23-2	18
5	Bicyclo[2.2.1]heptane-2,3-dione,...	166	C10H14O2	010334-26-6	18





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

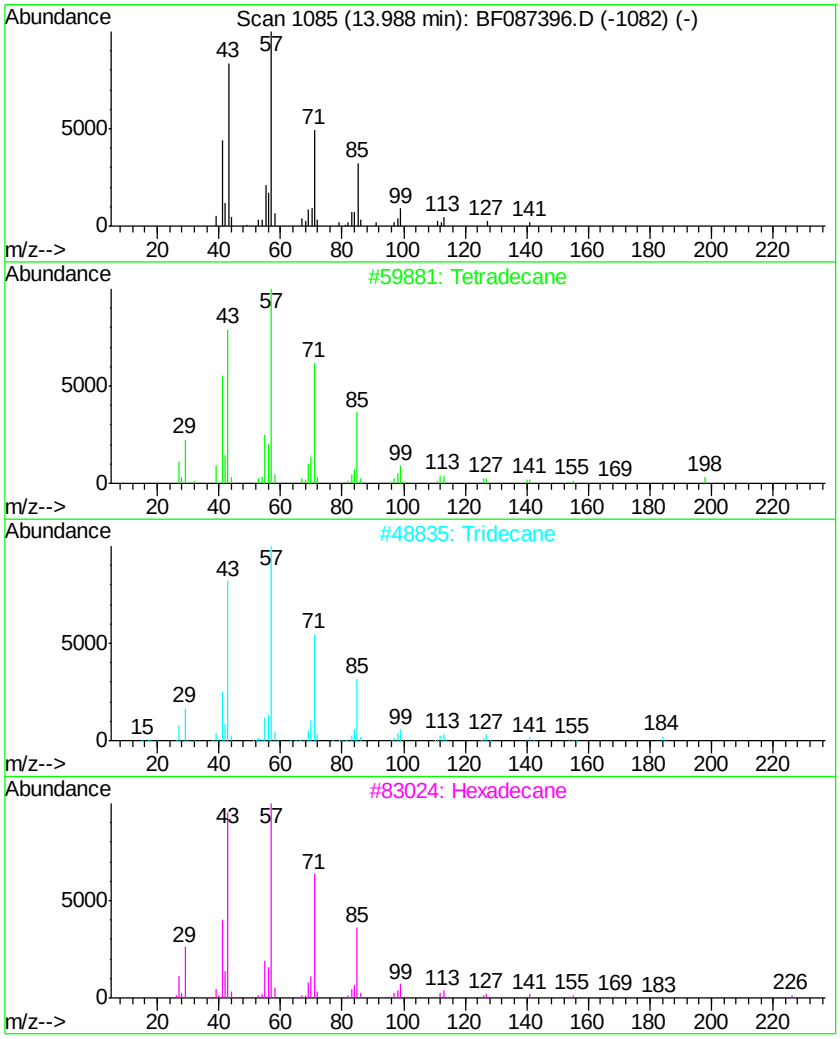
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

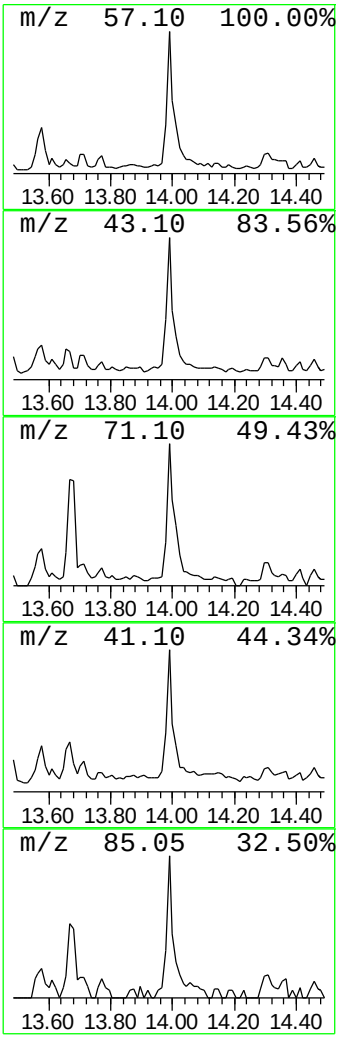
****

Peak Number 10 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	3.58 ng	115053	Phenanthrene-d10	14.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Pentadecane	212	C15H32	000629-62-9	86
5	Octadecane	254	C18H38	000593-45-3	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

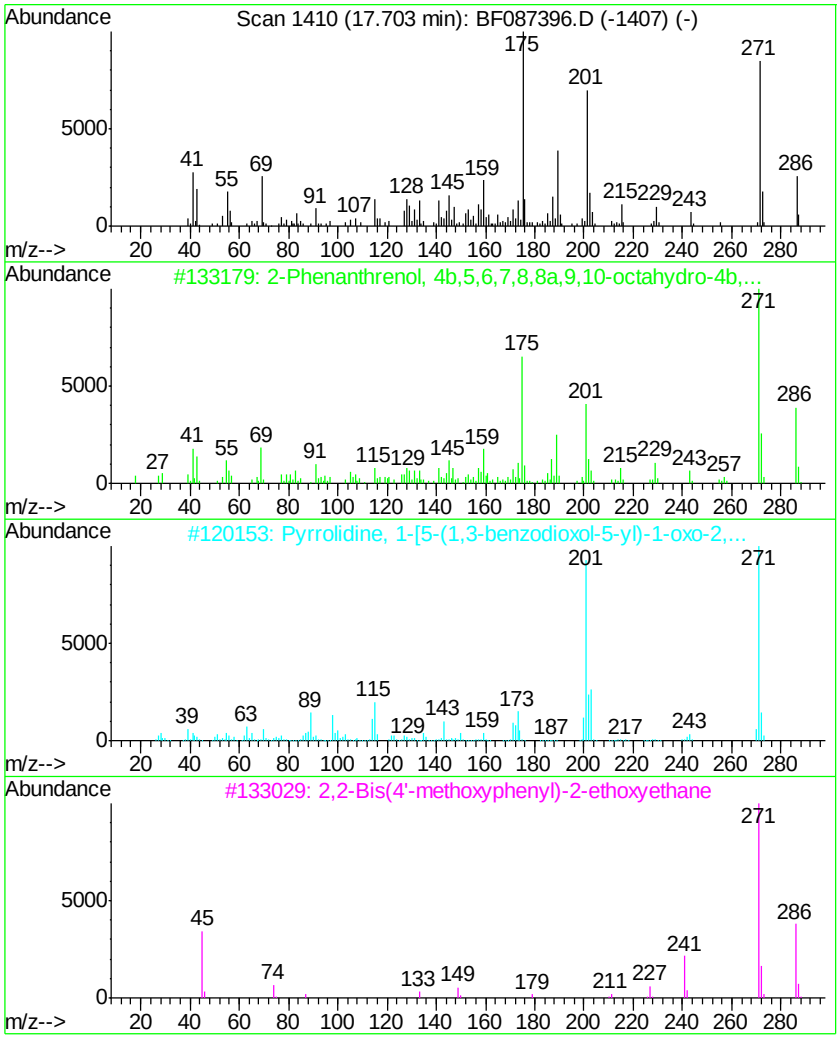
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

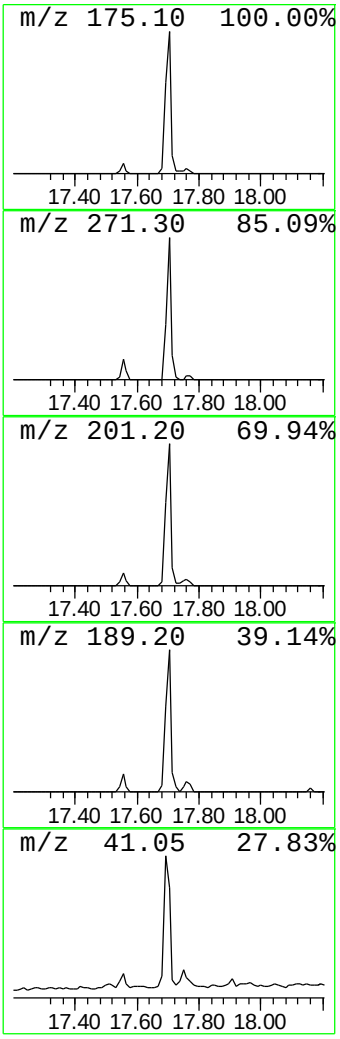
****

Peak Number 11 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.70	12.66 ng	394070	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	96
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	42
3	2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	22
4	2-Hexylquinolin-4-ol, 1-oxide	245	C15H19NO2	1000211-05-5	22
5	(+)-4-Methoxy-6-ketomorphinan	271	C17H21NO2	1000129-08-5	20





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Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

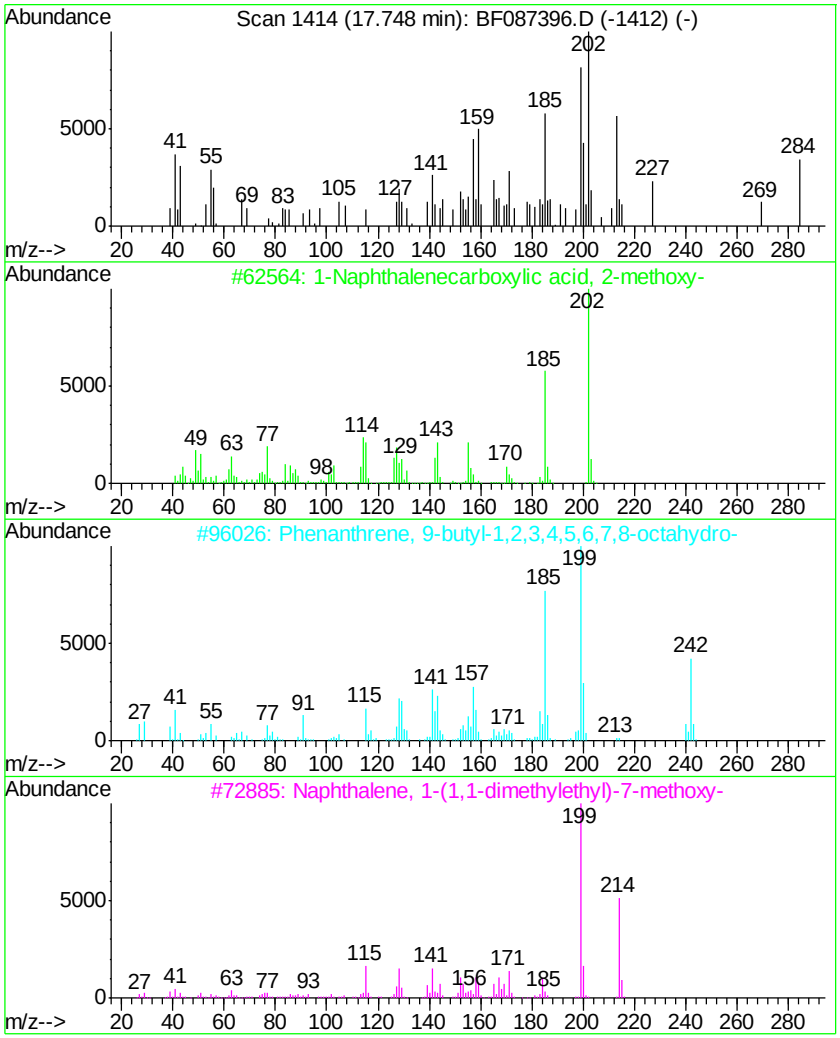
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

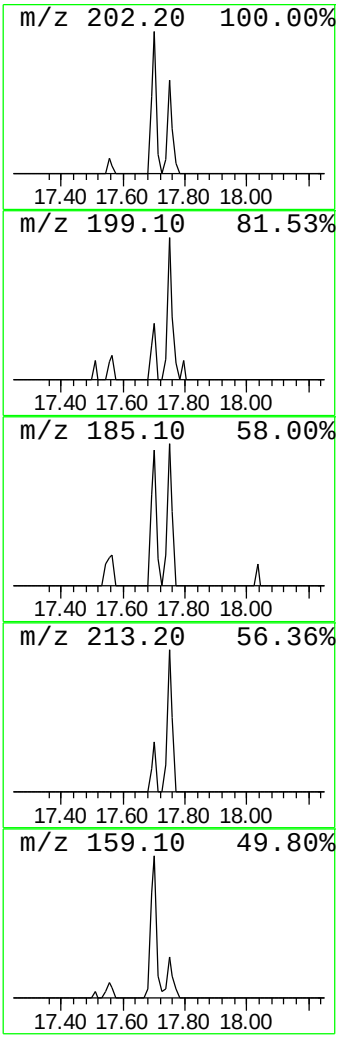
****

Peak Number 12 unknown17.75 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	2.12 ng	65950	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid, 2-...	202	C12H10O3	000947-62-6	35
2	Phenanthrene, 9-butyl-1,2,3,4,5,...	242	C18H26	016703-29-0	25
3	Naphthalene, 1-(1,1-dimethylethy...	214	C15H18O	060683-42-3	25
4	4-Chloro-3-ethyl-1,3-benzothiazo...	213	C9H8ClNOS	1000331-84-8	25
5	1H-Pyrazole-4-carbaldehyde, 5-hy...	202	C11H10N2O2	1000302-68-8	18





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Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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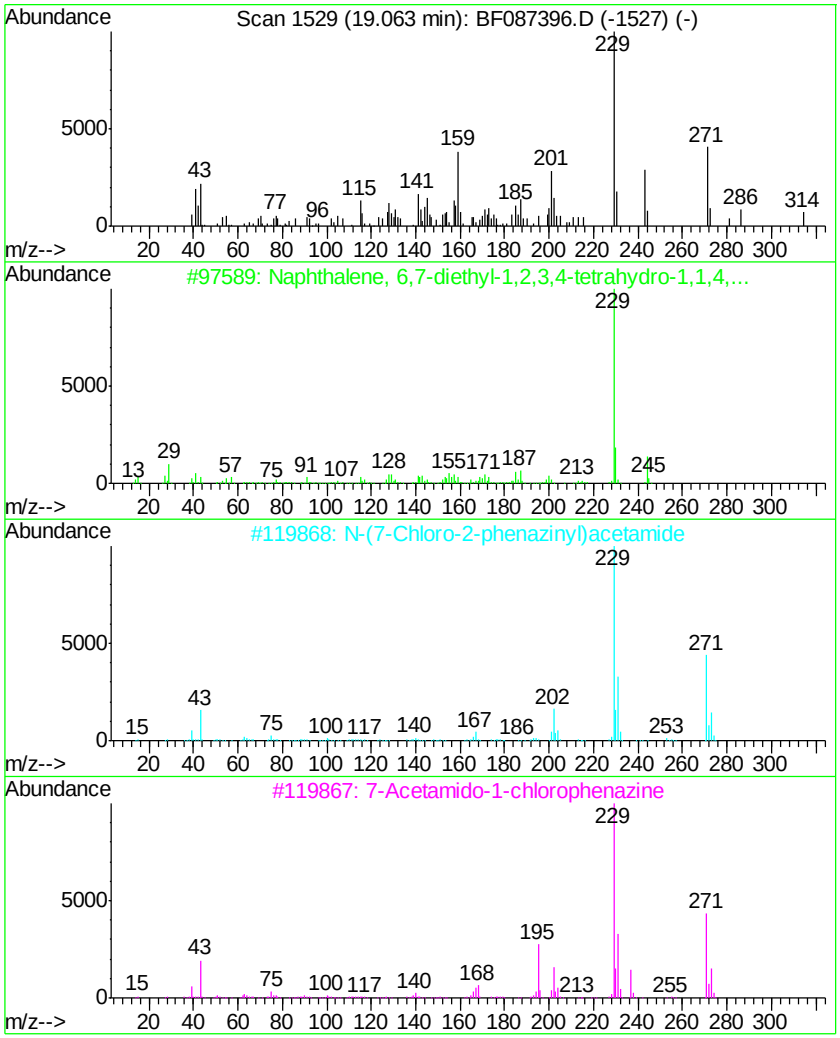
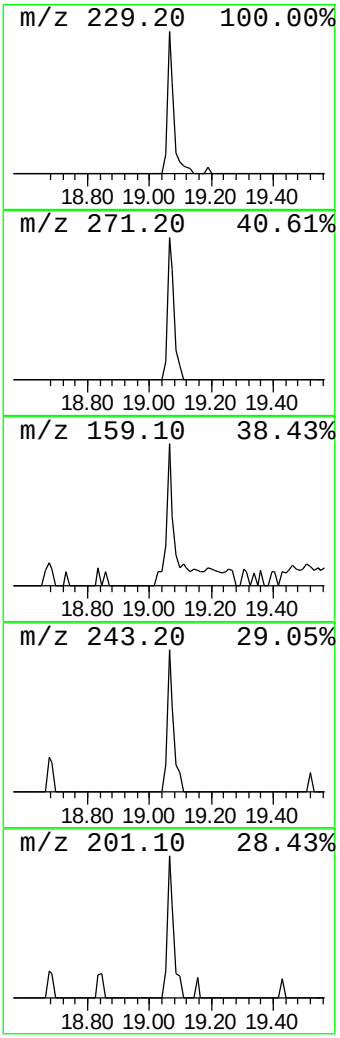
Peak Number 13 Naphthalene, 6,7-diethyl-1,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.06	2.72 ng	84601	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 6,7-diethyl-1,2,3,4...	244	C18H28	055741-10-1	52
2	N-(7-Chloro-2-phenazinyl)acetamide	271	C14H10ClN3O	023677-13-6	49
3	7-Acetamido-1-chlorophenazine	271	C14H10ClN3O	023677-12-5	49
4	1,2,3,4-Tetrahydro-7-methoxy-3-m...	229	C14H15NO2	032550-51-9	46
5	5-Amino-2-(1-methylethyl)-1-pent...	271	C15H21N5	1000326-95-8	43





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Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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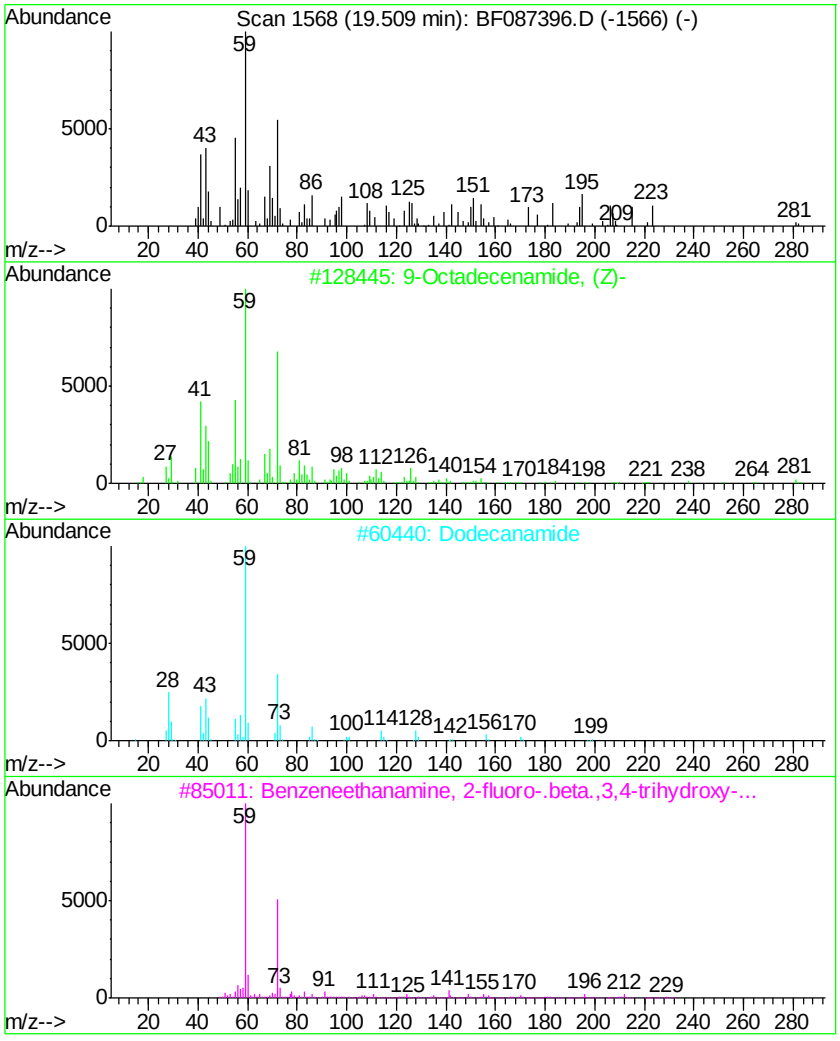
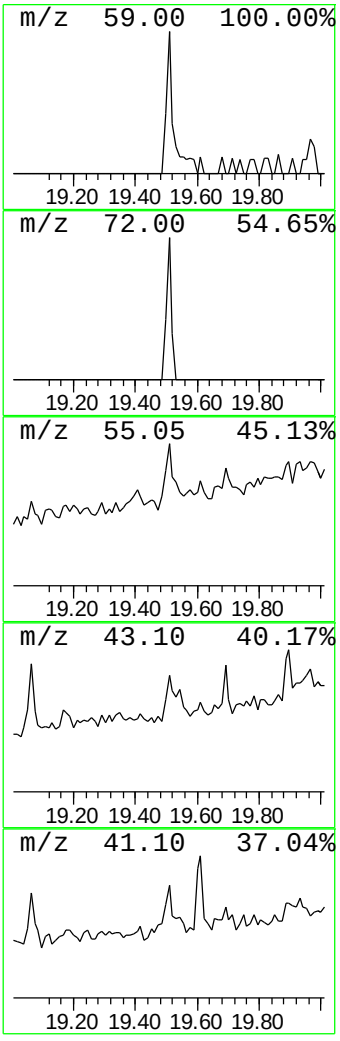
Peak Number 14 9-Octadecenamide, (Z)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.51	2.69 ng	56289	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	60
2	Dodecanamide	199	C12H25NO	001120-16-7	38
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	38
4	Tetradecanamide	227	C14H29NO	000638-58-4	38
5	Nonanamide	157	C9H19NO	001120-07-6	38





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
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Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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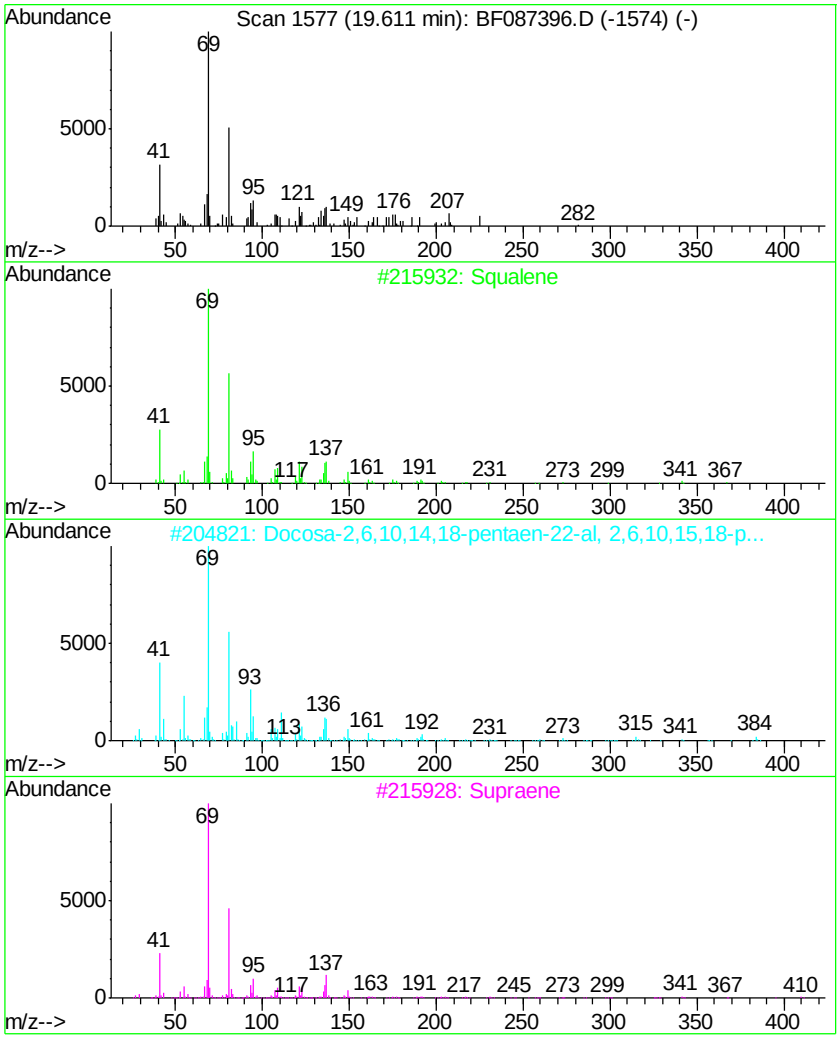
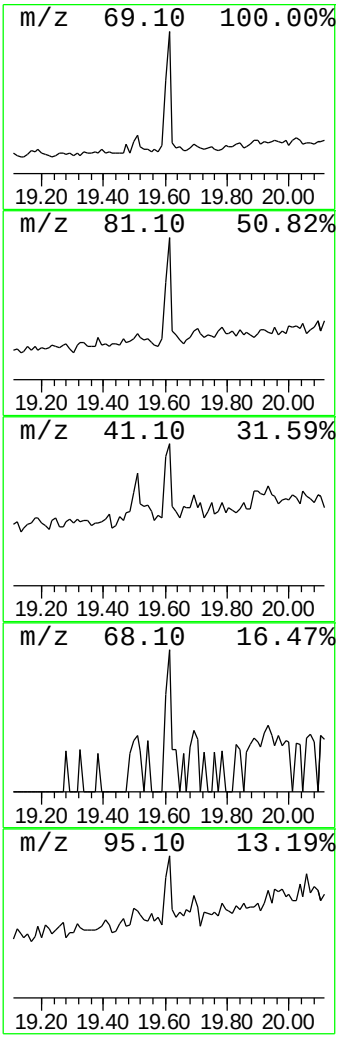
Peak Number 15 Squalene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	2.14 ng	44940	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	74
2	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
3	Supraene	410	C30H50	007683-64-9	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
5	2,6-Octadien-1-ol, 3,7-dimethyl-...	154	C10H18O	000106-25-2	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052516\
Data File : BF087396.D
Acq On : 26 May 2016 5:20
Operator : UM/SJ
Sample : H3220-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-34-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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...	4.80	13.3	ng	454564	1	7.52	686136	20.0
unknown7.19	7.19	115.7	ng	3968590	1	7.52	686136	20.0
Cycloisolongifole...	11.69	3.2	ng	126762	3	12.38	795644	20.0
4,5-di-epi-aristo...	11.77	6.1	ng	243911	3	12.38	795644	20.0
.beta.-ylangene	11.82	2.8	ng	110772	3	12.38	795644	20.0
Bicyclo[3.1.1]hep...	12.31	3.0	ng	117979	3	12.38	795644	20.0
unknown13.47	13.47	5.8	ng	231825	3	12.38	795644	20.0
Tetradecane	13.99	3.6	ng	115053	4	14.78	643006	20.0
2-Phenanthrenol, ...	17.70	12.7	ng	394070	5	18.47	622433	20.0
unknown17.75	17.75	2.1	ng	65950	5	18.47	622433	20.0
Naphthalene, 6,7-...	19.06	2.7	ng	84601	5	18.47	622433	20.0
9-Octadecenamide,...	19.51	2.7	ng	56289	6	20.14	419242	20.0
Squalene	19.61	2.1	ng	44940	6	20.14	419242	20.0