LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087400.D
Acq On : 26 May 2016 7:35
Operator : UM/SJ
Sample : H3220-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-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	4	5	54	rVB	2757373	5407056	100.00%	14.480%
2	4.787	277	280	297	rBV	176351	514708	9.52%	1.378%
3	5.450	335	338	359	rBV	2416897	4031878	74.57%	10.797%
4	7.084	478	481	484	rBV	2291619	3941537	72.90%	10.555%
5	7.187	487	490	502	rVB	2904517	4194153	77.57%	11.232%
6	7.519	517	519	525	rBV	553081	689110	12.74%	1.845%
7	7.759	537	540	543	rBV	2394742	2941799	54.41%	7.878%
8	8.433	596	599	602	rBV	1590436	2473261	45.74%	6.623%
9	9.553	694	697	711	rBV	623356	820244	15.17%	2.197%
10	11.336	849	853	855	rBV	2773681	3839567	71.01%	10.282%
11	12.022	910	913	916	rBV	724773	846948	15.66%	2.268%
12	12.376	941	944	955	rVB	622878	761280	14.08%	2.039%
13	13.668	1054	1057	1060	rBV	1249229	1899147	35.12%	5.086%
14	13.988	1082	1085	1093	rBV	52680	91718	1.70%	0.246%
15	14.777	1151	1154	1161	rVB	523756	638533	11.81%	1.710%
16	17.131	1357	1360	1363	rBV	2593586	2829881	52.34%	7.578%
17	18.388	1467	1470	1474	rBV	38119	72450	1.34%	0.194%
18	18.468	1474	1477	1480	rVV	562076	627273	11.60%	1.680%
19	18.537	1480	1483	1486	rVB	62557	100504	1.86%	0.269%
20	19.509	1565	1568	1569	rBV	38476	61518	1.14%	0.165%
21	19.611	1574	1577	1579	rVV	90604	122053	2.26%	0.327%
22	20.137	1621	1623	1629	rBV	348824	437510	8.09%	1.172%

Sum of corrected areas: 37342128

LSC Report - Integrated Chromatogram

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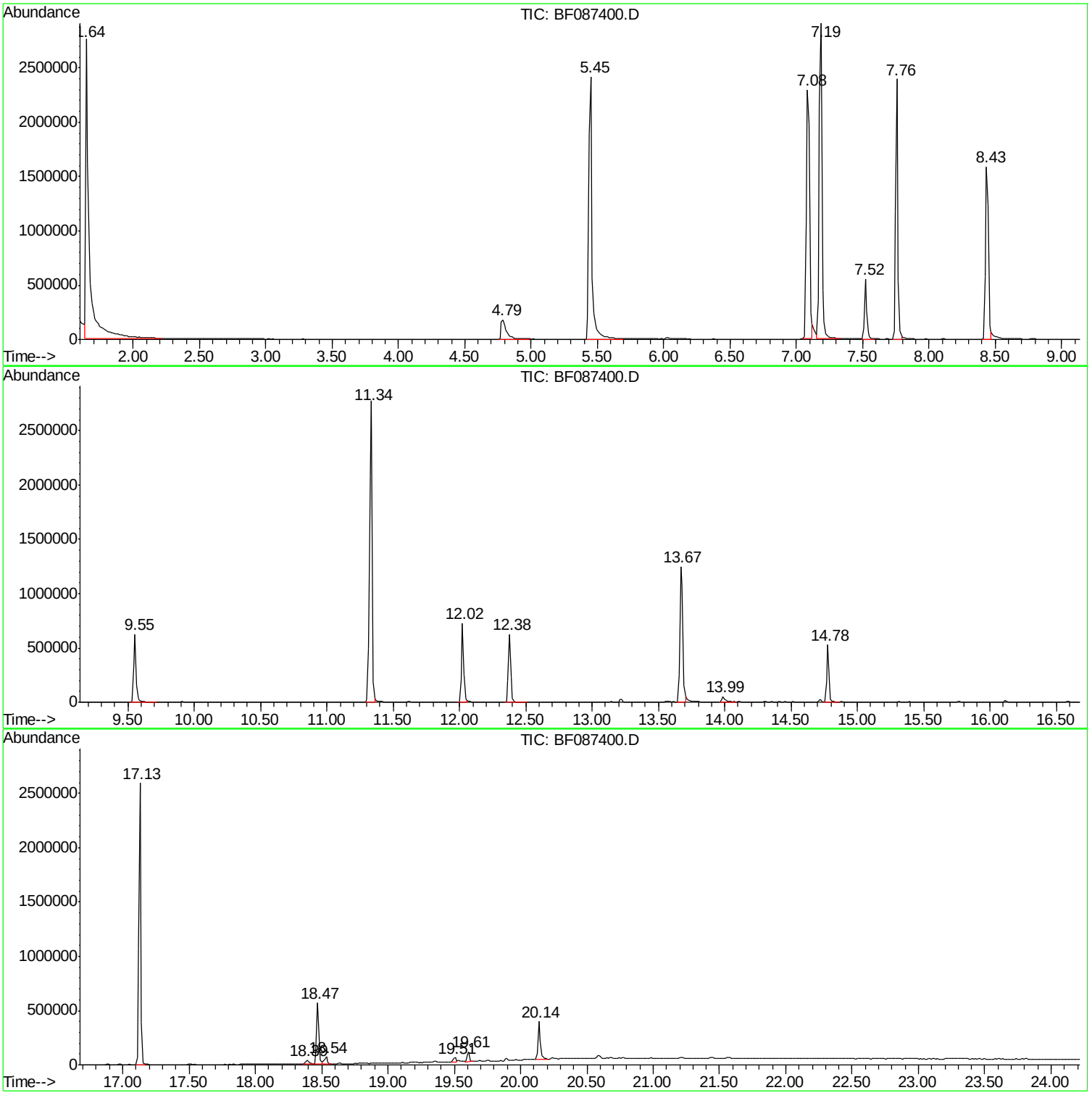
Instrument : BNA_F
ClientSampleId : SB-27-COMP

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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Data File : BF087400.D
Acq On : 26 May 2016 7:35
Operator : UM/SJ
Sample : H3220-12
Misc :
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Instrument : BNA_F
ClientSampleId : SB-27-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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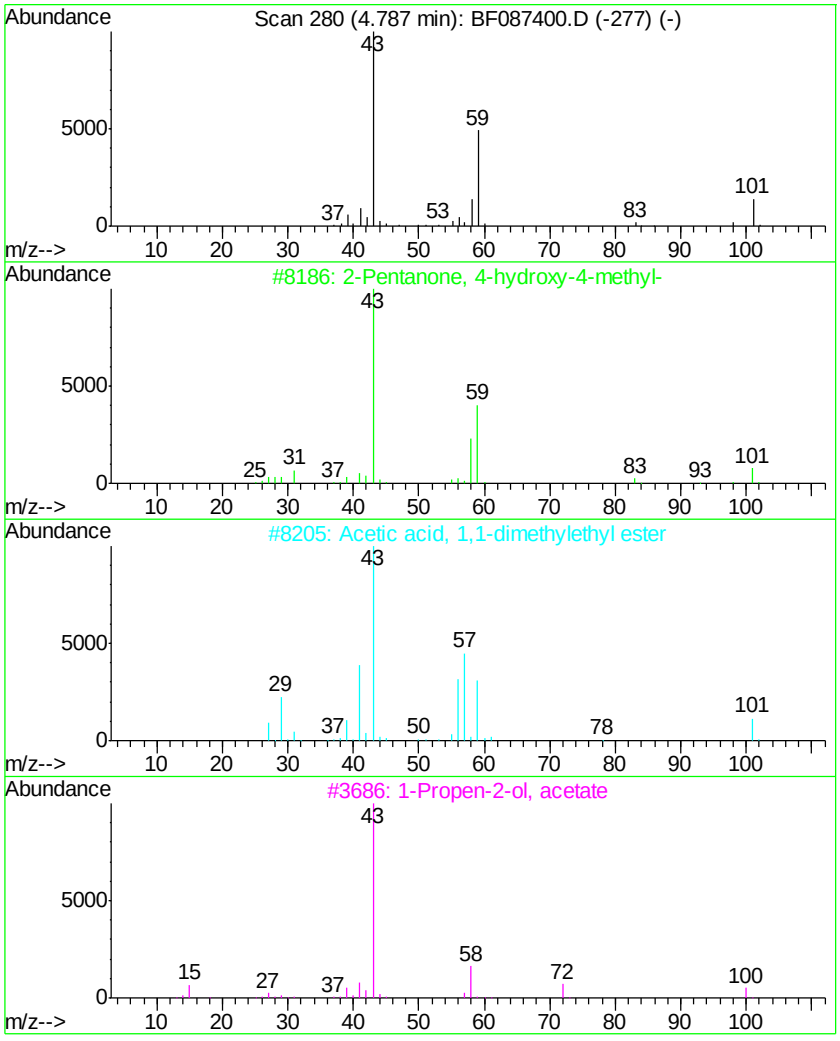
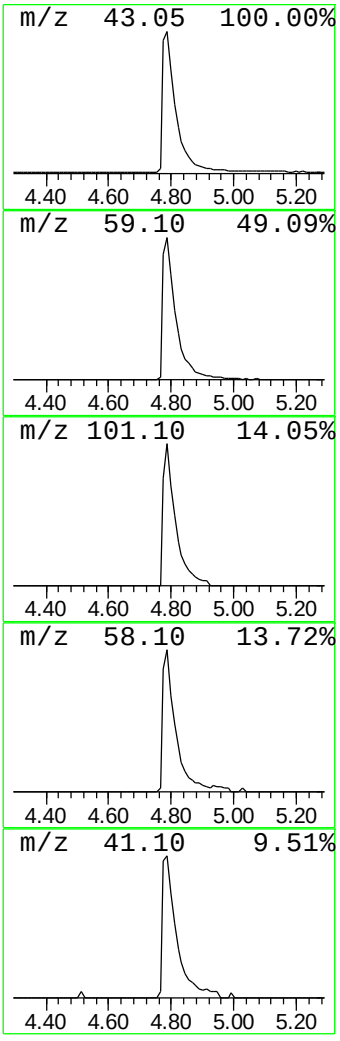
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	14.94 ng	514708	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	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane	58	C4H10	000106-97-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087400.D
Acq On : 26 May 2016 7:35
Operator : UM/SJ
Sample : H3220-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-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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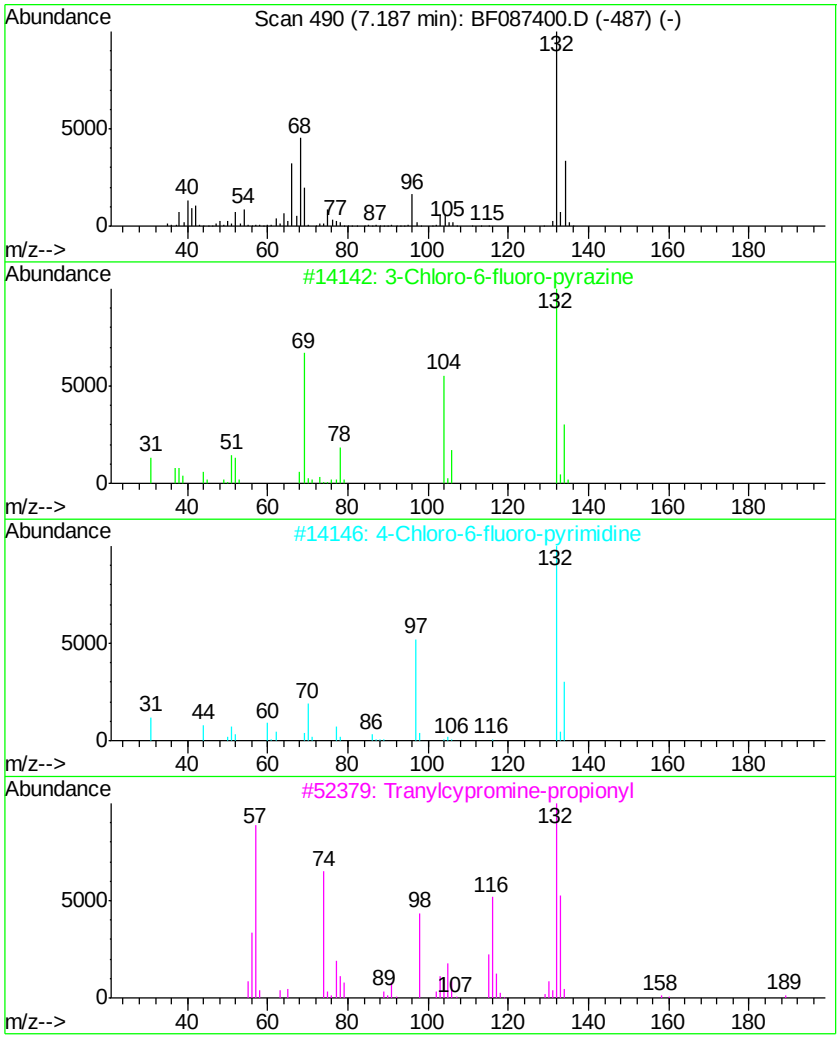
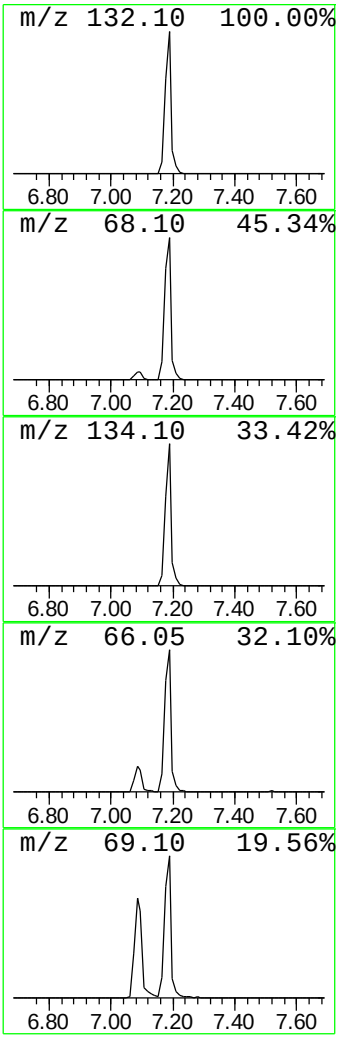
Peak Number 3 unknown7.19 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	121.73 ng	4194150	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	16





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Operator : UM/SJ
Sample : H3220-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-27-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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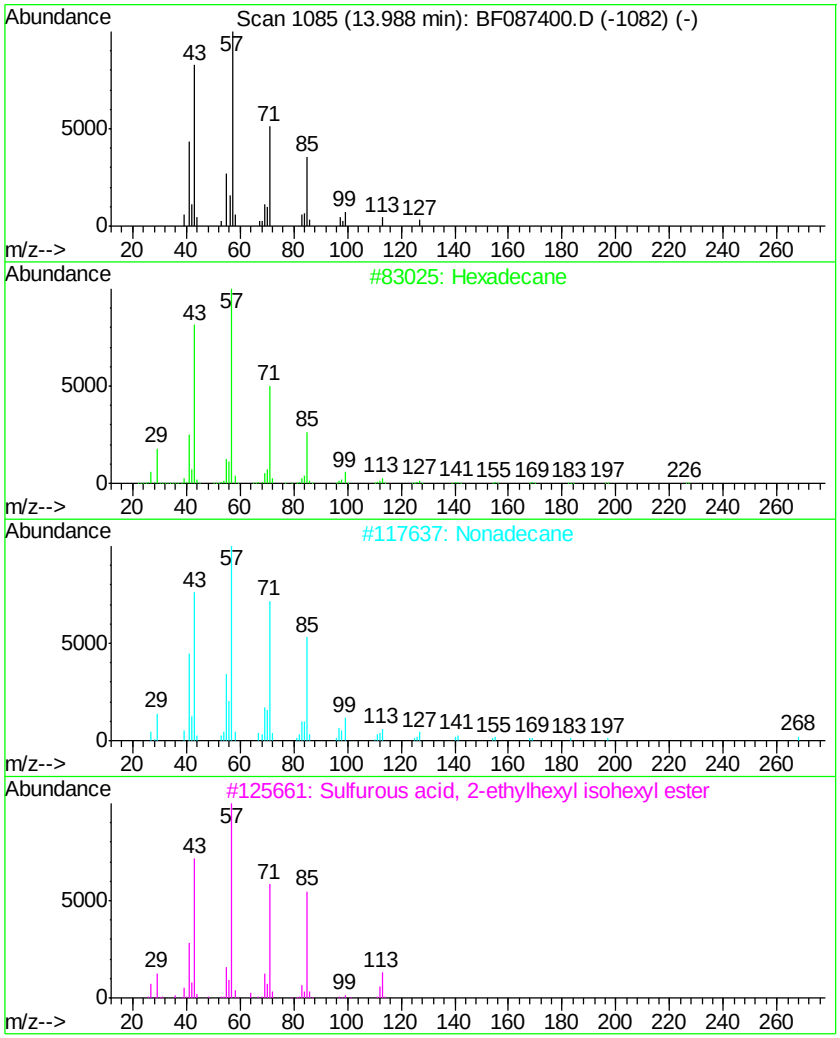
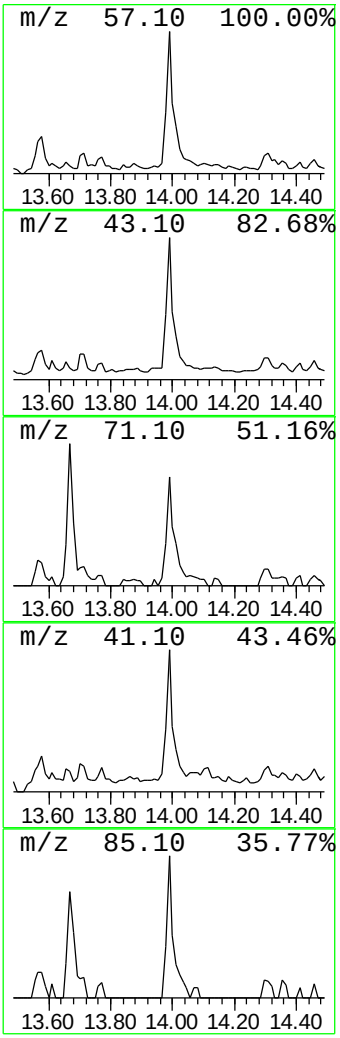
Peak Number 5 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	2.87 ng	91718	Phenanthrene-d10	14.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Nonadecane	268	C19H40	000629-92-5	80
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	78
4	Eicosane	282	C20H42	000112-95-8	72
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64





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Instrument : BNA_F
ClientSampleId : SB-27-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
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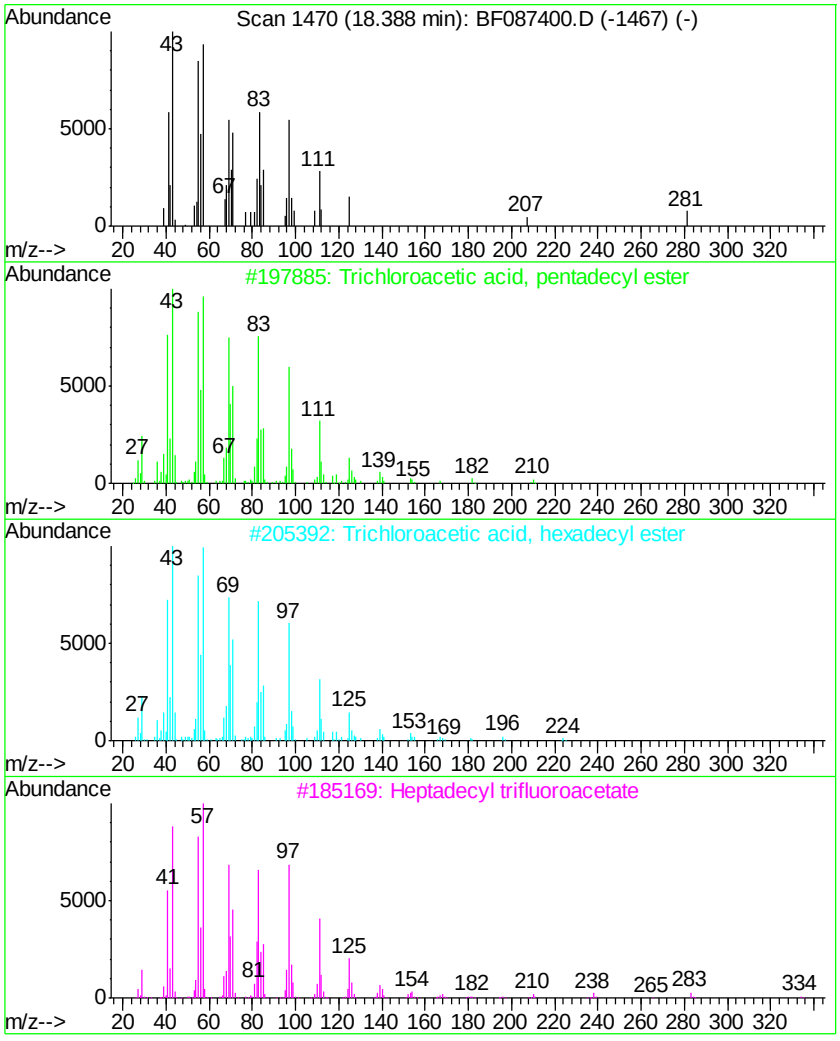
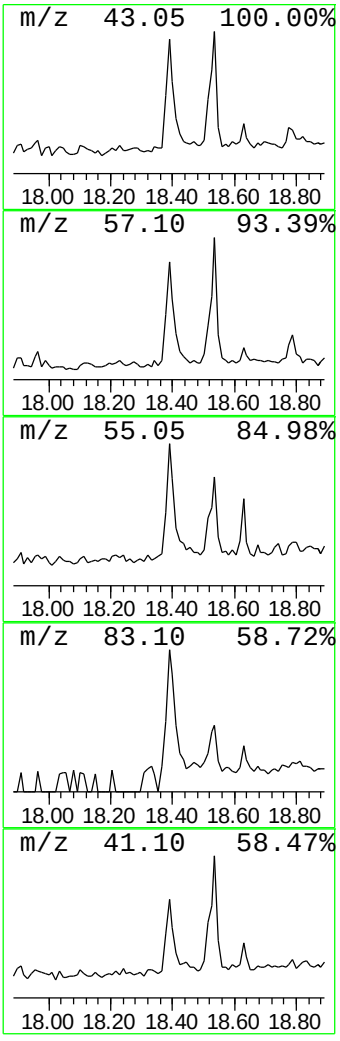
Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.31 ng	72450	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





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Instrument : BNA_F
ClientSampleId : SB-27-COMP

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

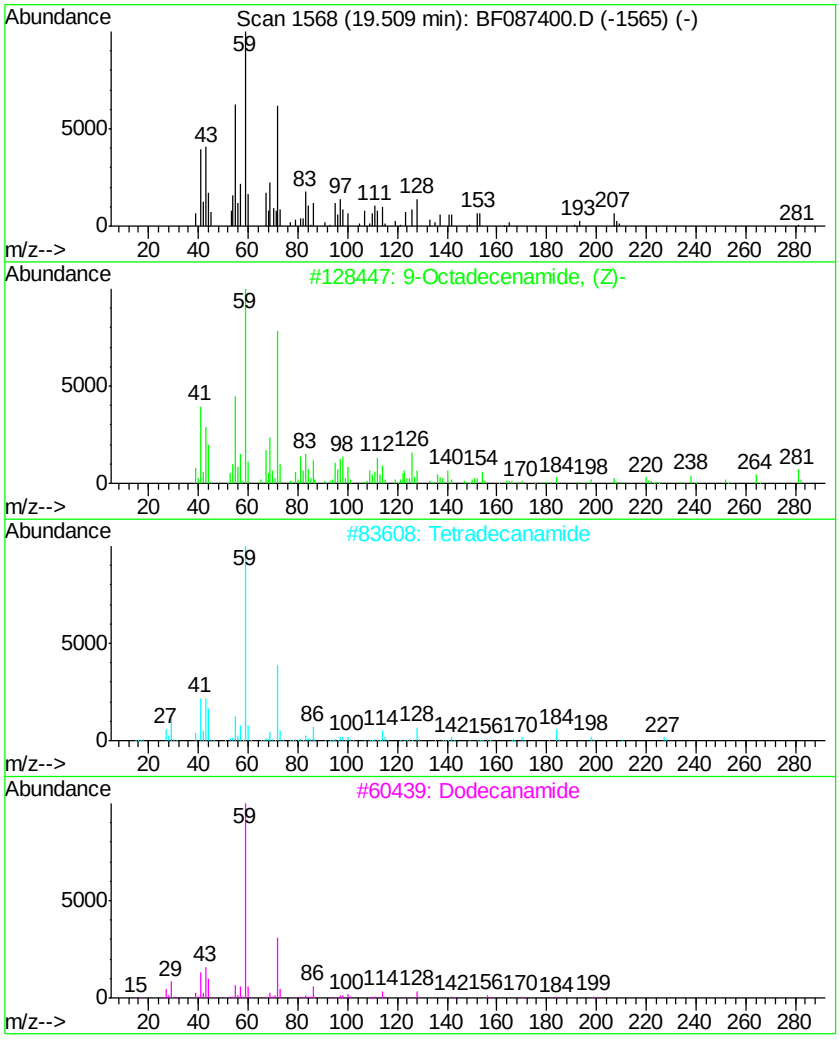
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

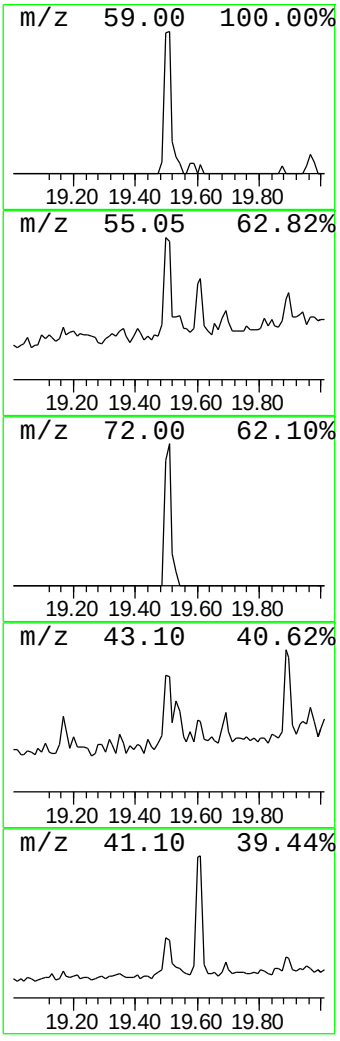
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.51	2.81 ng	61518	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	64
3	Dodecanamide	199	C12H25NO	001120-16-7	59
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	50
5	d-Glucosamine	179	C6H13NO5	000090-77-7	50





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Instrument : BNA_F
ClientSampleId : SB-27-COMP

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

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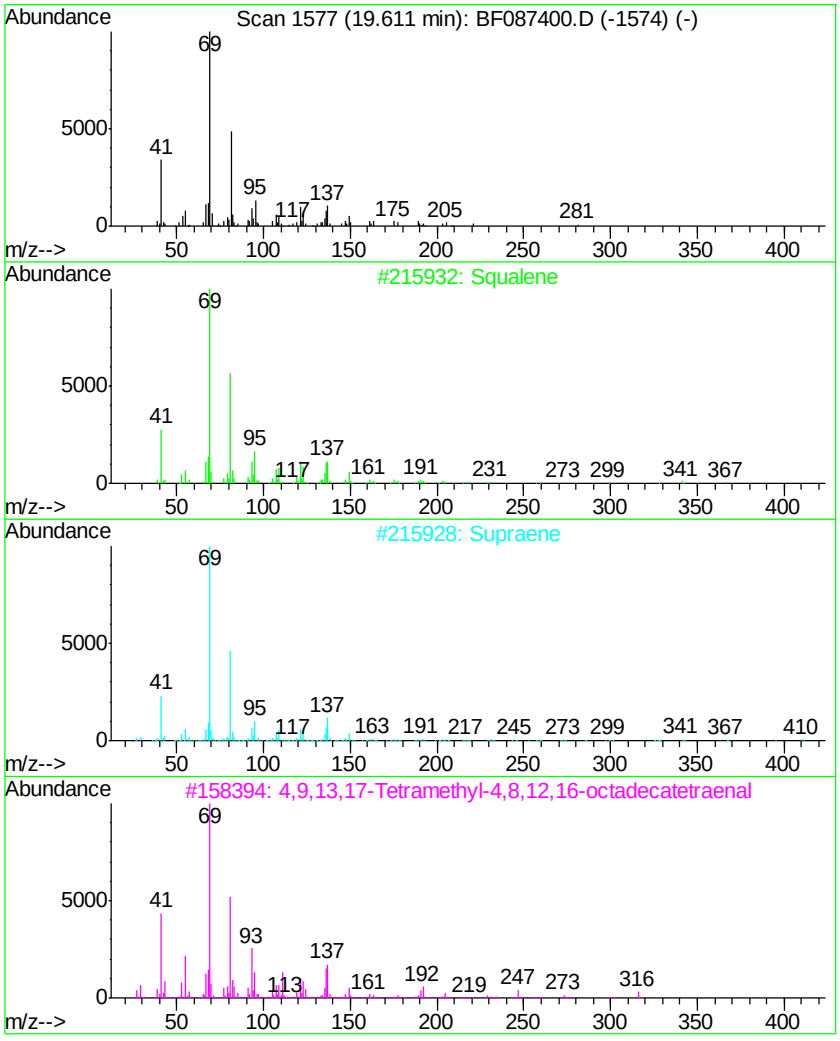
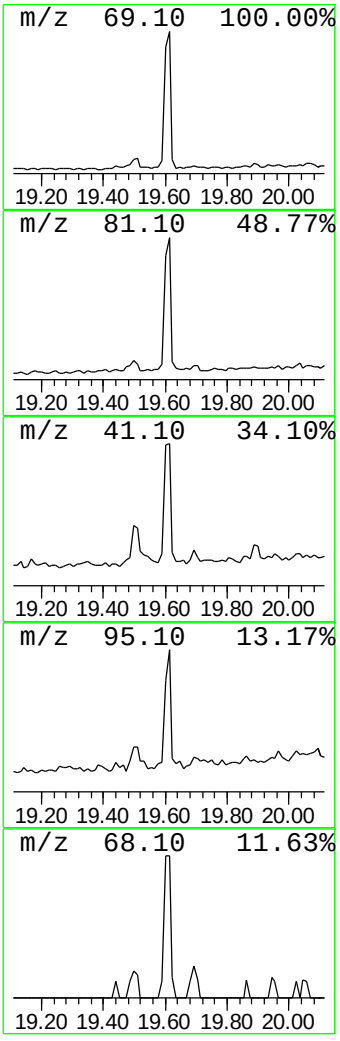
Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	5.58 ng	122053	Perylene-d12	20.14

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	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	64





Tentatively Identified Compound (LSC) summary

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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...	4.79	14.9	ng	514708	1	7.52	689110	20.0
unknown7.19	7.19	121.7	ng	4194150	1	7.52	689110	20.0
Hexadecane	13.99	2.9	ng	91718	4	14.78	638533	20.0
Trichloroacetic a...	18.39	2.3	ng	72450	5	18.47	627273	20.0
9-Octadecenamide,...	19.51	2.8	ng	61518	6	20.14	437510	20.0
Squalene	19.61	5.6	ng	122053	6	20.14	437510	20.0