LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087870.D
Acq On : 10 Jun 2016 13:06
Operator : UM/SJ
Sample : H3426-14
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-58

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-BF060716.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	1.747	12	14	23	rVB	273438	552982	9.25%	1.882%
2	1.873	23	25	73	rVB	2574399	5977411	100.00%	20.340%
3	4.981	295	297	305	rVB	142629	177709	2.97%	0.605%
4	5.404	331	334	336	rBV	1852047	1927057	32.24%	6.557%
5	6.444	422	425	427	rBV	1825782	1925424	32.21%	6.552%
6	6.582	434	437	439	rBV	1540285	2089893	34.96%	7.112%
7	6.810	454	457	459	rBV	903094	743685	12.44%	2.531%
8	6.970	468	471	473	rVB	1675178	1729983	28.94%	5.887%
9	7.370	503	506	509	rBV	1005586	1271690	21.27%	4.327%
10	7.462	512	514	516	rBV	173062	136515	2.28%	0.465%
11	8.102	567	570	572	rBV	836683	963570	16.12%	3.279%
12	9.176	661	664	666	rBV	2831719	2745552	45.93%	9.343%
13	9.485	689	691	693	rBV	83618	67351	1.13%	0.229%
14	9.565	696	698	700	rBV	238710	186785	3.12%	0.636%
15	9.850	720	723	725	rBV	1047440	1183659	19.80%	4.028%
16	10.628	789	791	794	rBV	1419023	1392345	23.29%	4.738%
17	11.325	850	852	854	rBV	1296562	1159679	19.40%	3.946%
18	12.422	946	948	951	rBV	149192	132572	2.22%	0.451%
19	12.731	973	975	979	rBV2	66475	122553	2.05%	0.417%
20	12.902	988	990	993	rBV	1862489	2143894	35.87%	7.295%
21	13.337	1025	1028	1029	rVV	258414	250485	4.19%	0.852%
22	13.371	1029	1031	1035	rVB2	94394	157563	2.64%	0.536%
23	13.805	1066	1069	1073	rBV	100116	143895	2.41%	0.490%
24	13.942	1079	1081	1084	rBV2	906445	976980	16.34%	3.324%
25	14.708	1145	1148	1152	rBV	201497	297094	4.97%	1.011%
26	15.360	1201	1205	1207	rBV	462164	708976	11.86%	2.413%
27	15.714	1232	1236	1242	rBV	18221	73540	1.23%	0.250%
28	15.851	1246	1248	1252	rBV	44916	79457	1.33%	0.270%
29	17.268	1368	1372	1376	rBV4	28514	69187	1.16%	0.235%

Sum of corrected areas: 29387486

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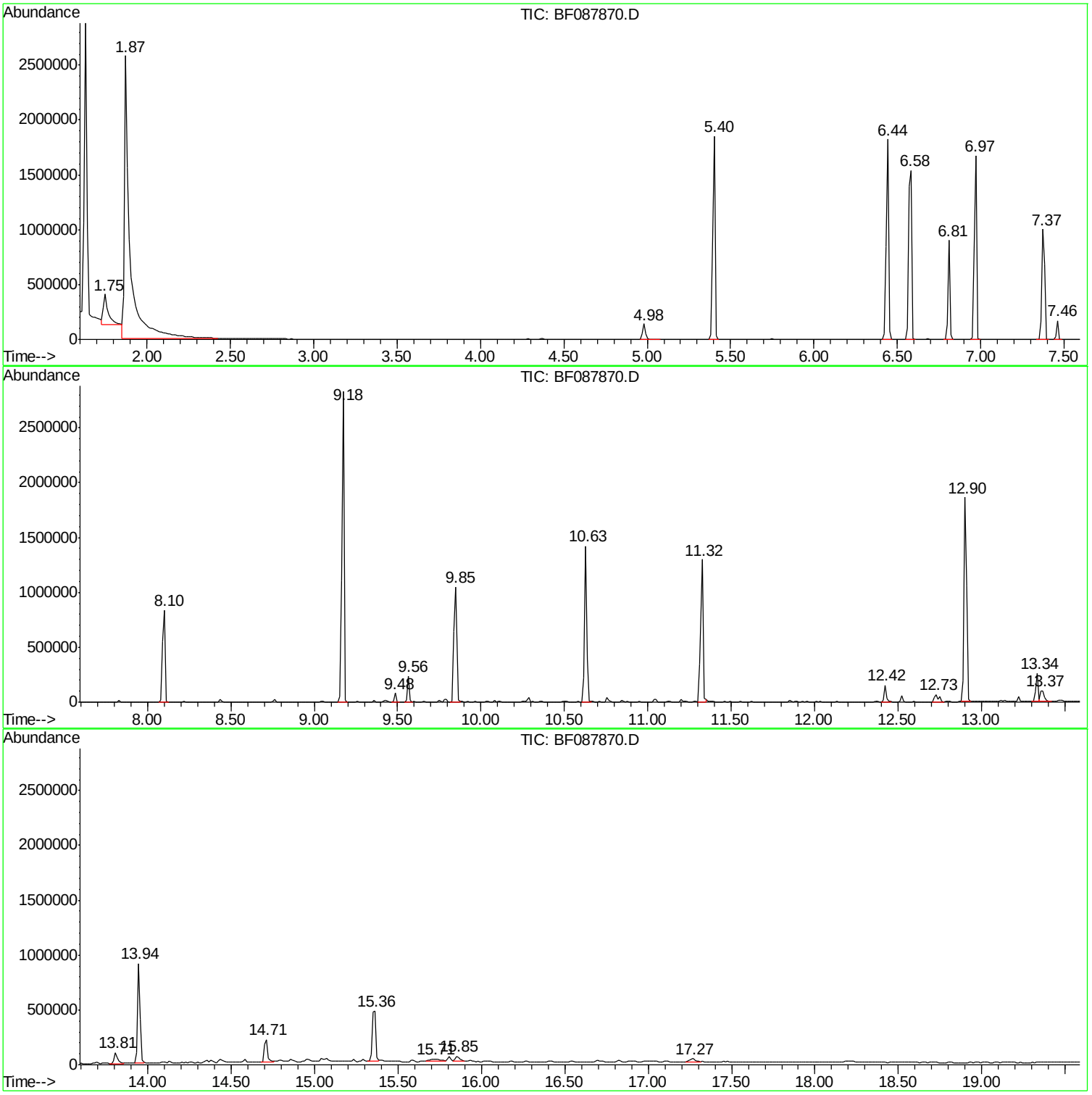
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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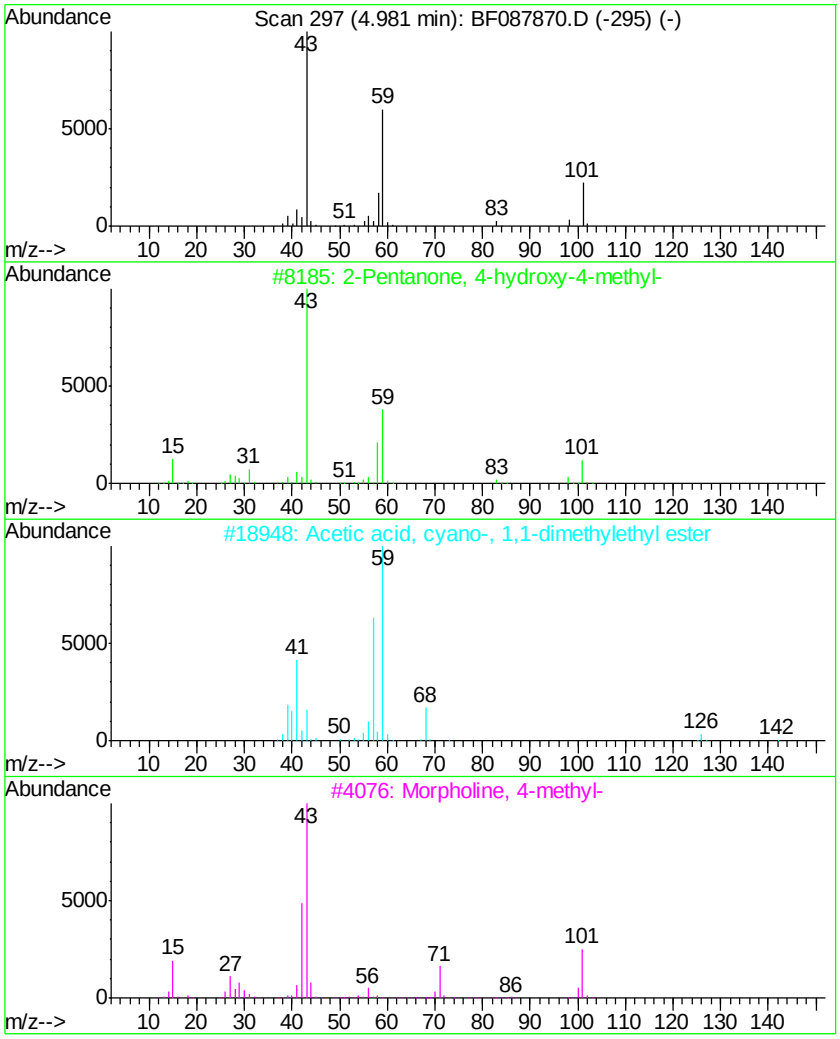
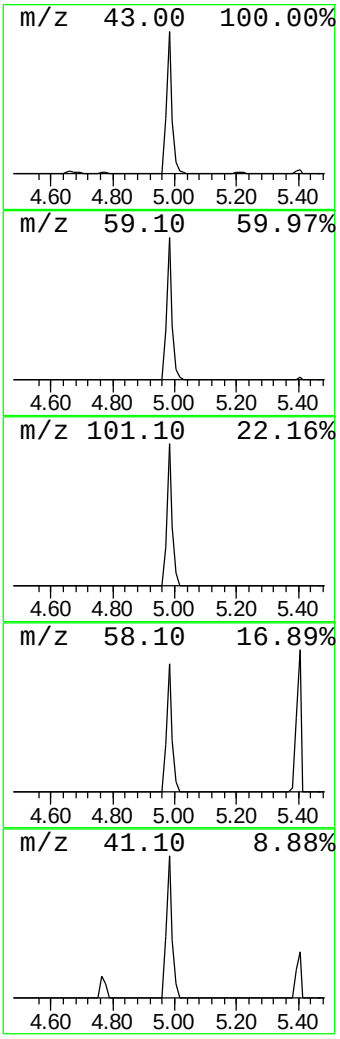
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	4.78 ng	177709	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Instrument : BNA_F
ClientSampleId : SS-58

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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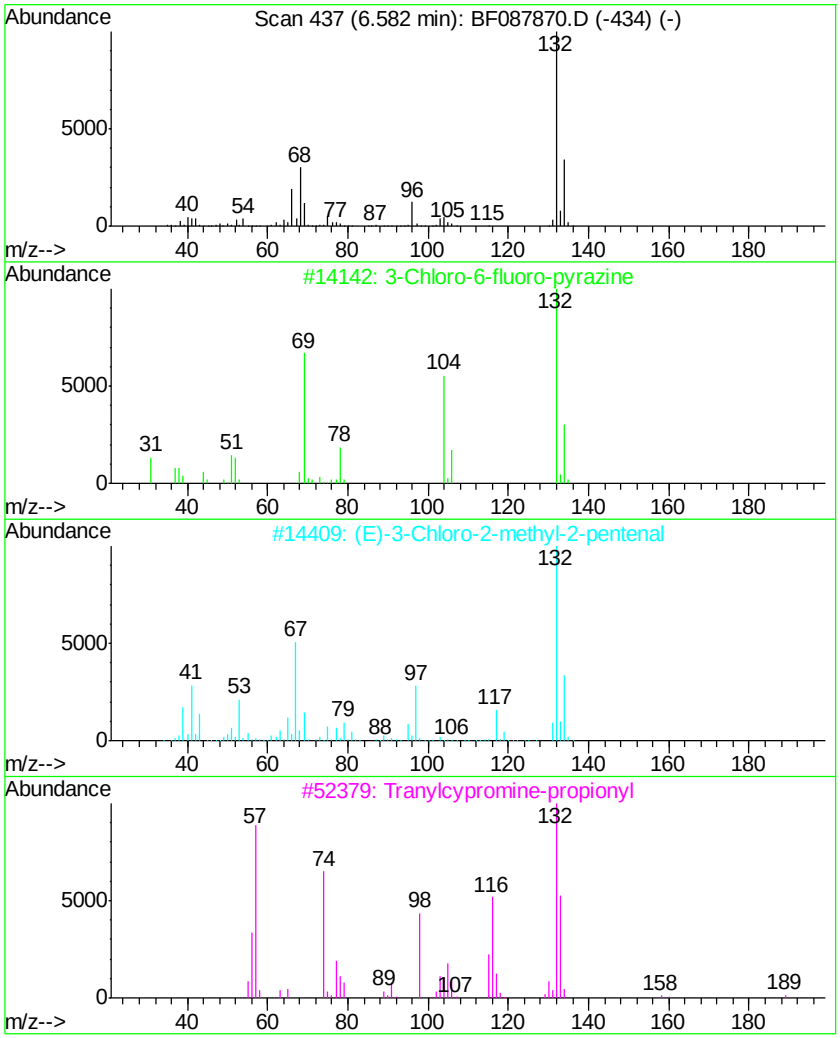
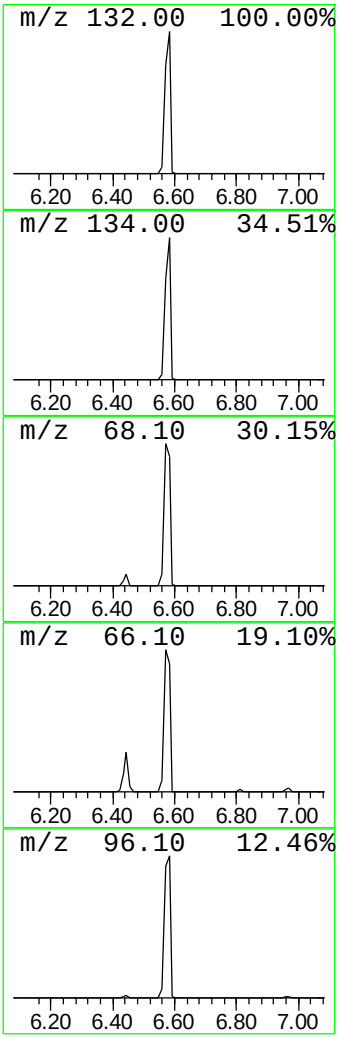
Peak Number 4 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	56.20 ng	2089890	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12
5	Amphetaminil	250	C17H18N2	017590-01-1	12





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Instrument : BNA_F
ClientSampleId : SS-58

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
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TIC Library : C:\Database\NIST11.L
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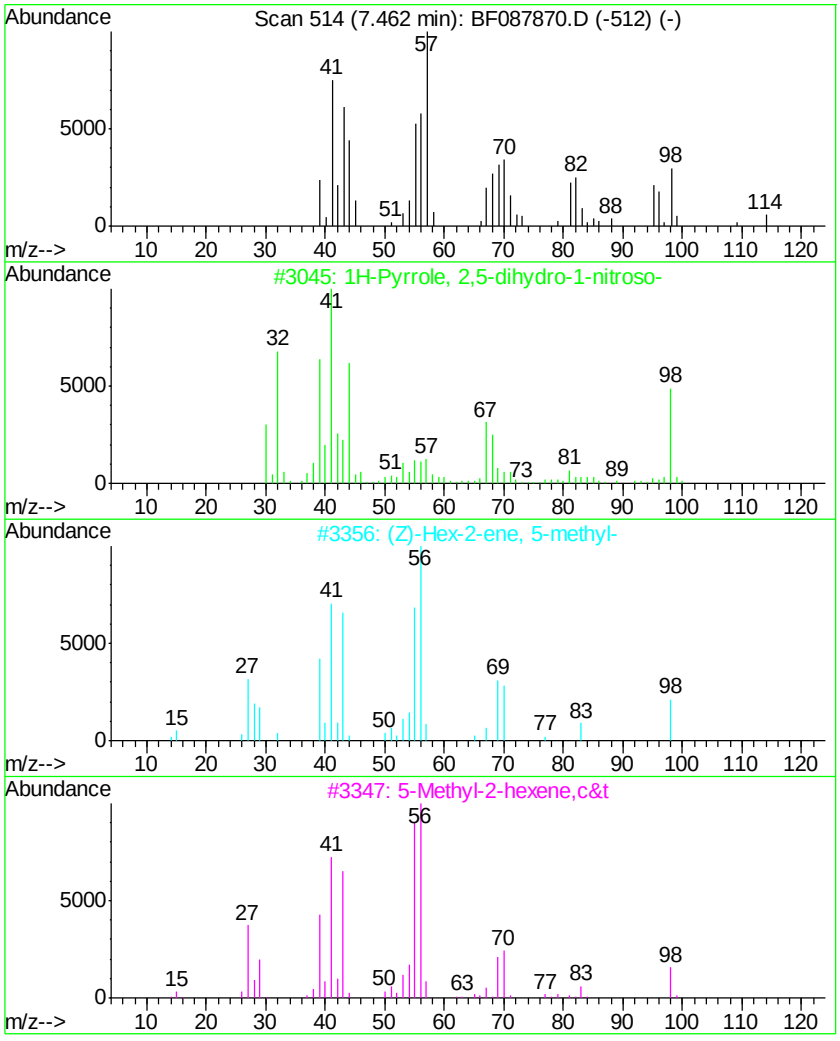
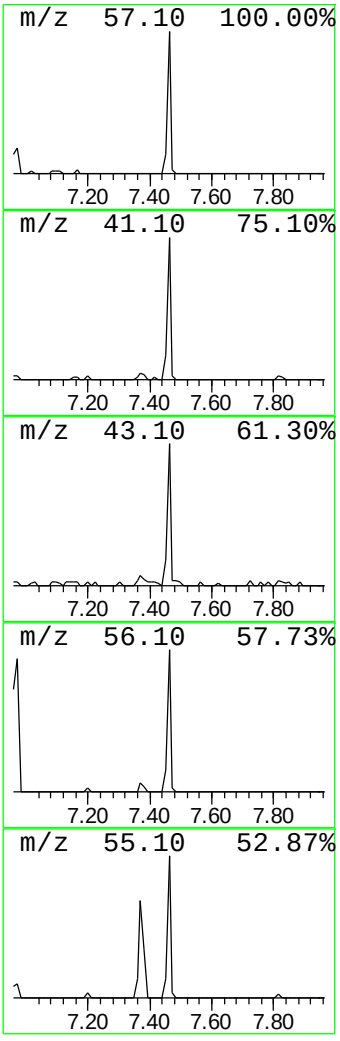
Peak Number 6 unknown7.46 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	2.83 ng	136515	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrole, 2,5-dihydro-1-nitroso-	98	C4H6N2O	010552-94-0	35
2	(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	27
3	5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	27
4	2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	27
5	(Z)-2-Heptene	98	C7H14	006443-92-1	25





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ClientSampleId : SS-58

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TIC Library : C:\Database\NIST11.L
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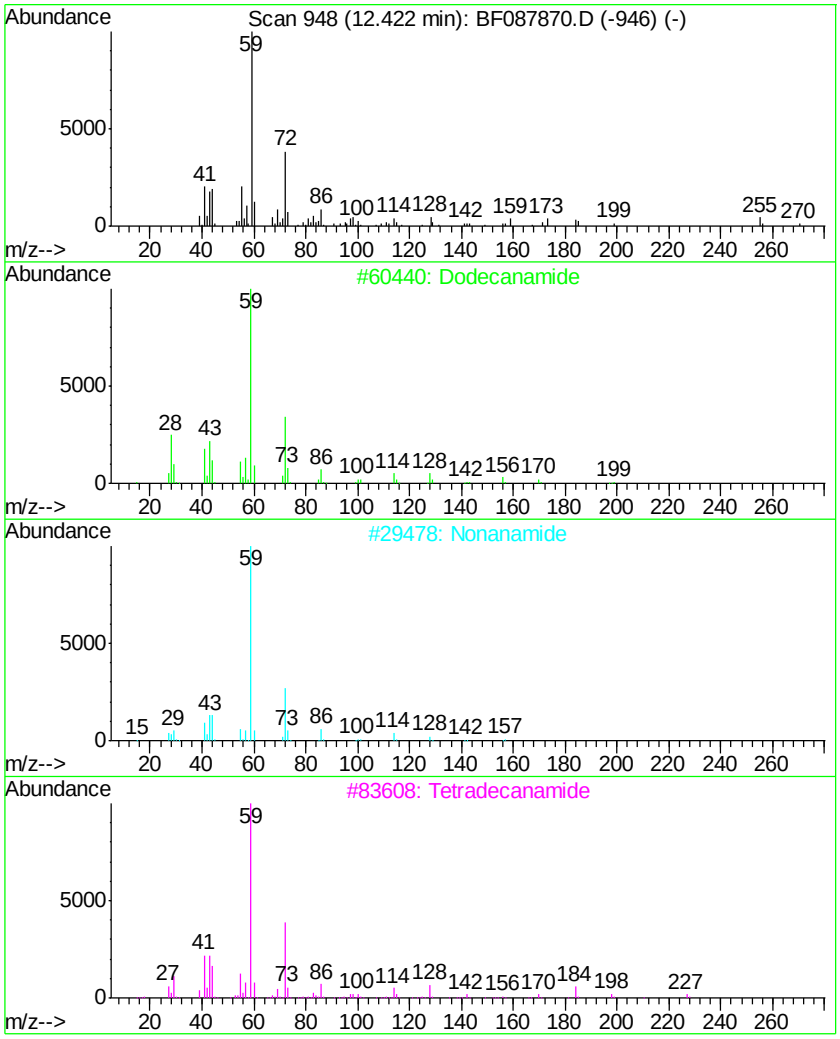
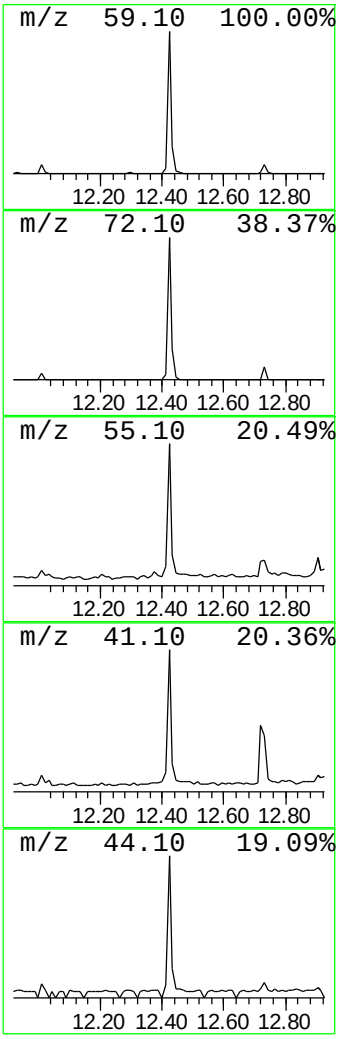
Peak Number 7 Dodecanamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	2.29 ng	132572	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanamide	199	C12H25NO	001120-16-7	90
2	Nonanamide	157	C9H19NO	001120-07-6	83
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Hexadecanamide	255	C16H33NO	000629-54-9	76
5	Decanamide-	171	C10H21NO	002319-29-1	74





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Instrument : BNA_F
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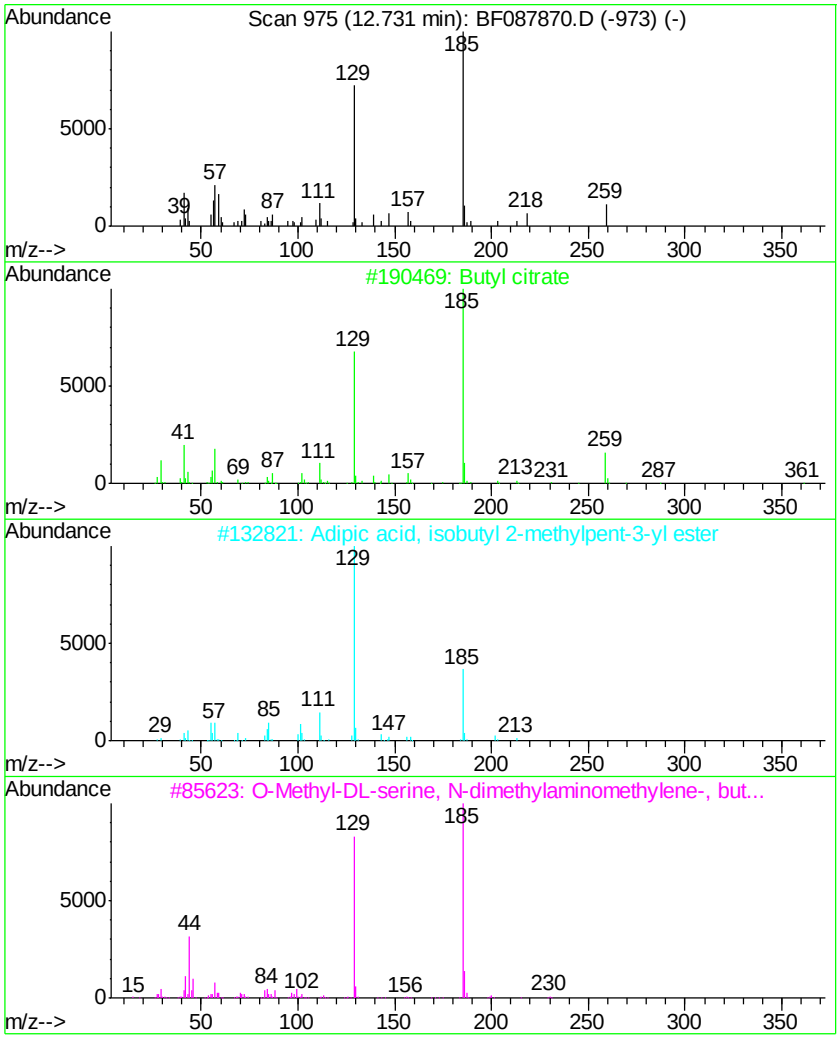
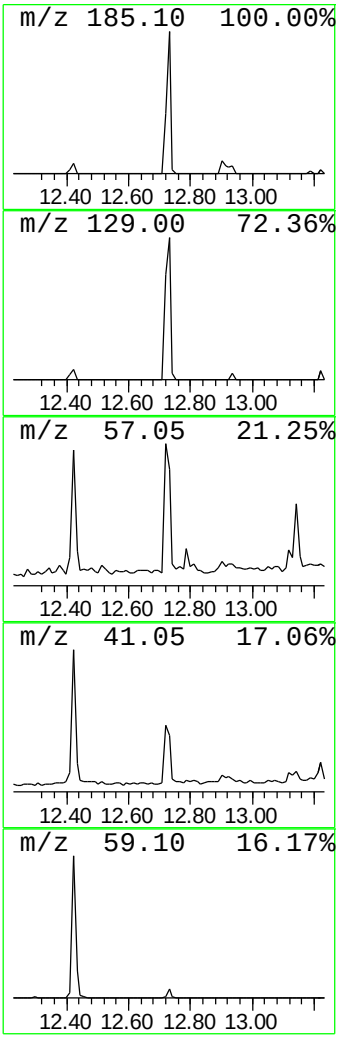
Peak Number 8 Butyl citrate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.51 ng	122553	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	87
2	Adipic acid, isobutyl 2-methylpe...	286	C16H30O4	1000353-55-7	64
3	O-Methyl-DL-serine, N-dimethylam...	230	C11H22N2O3	1000375-99-5	53
4	Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	50
5	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	50





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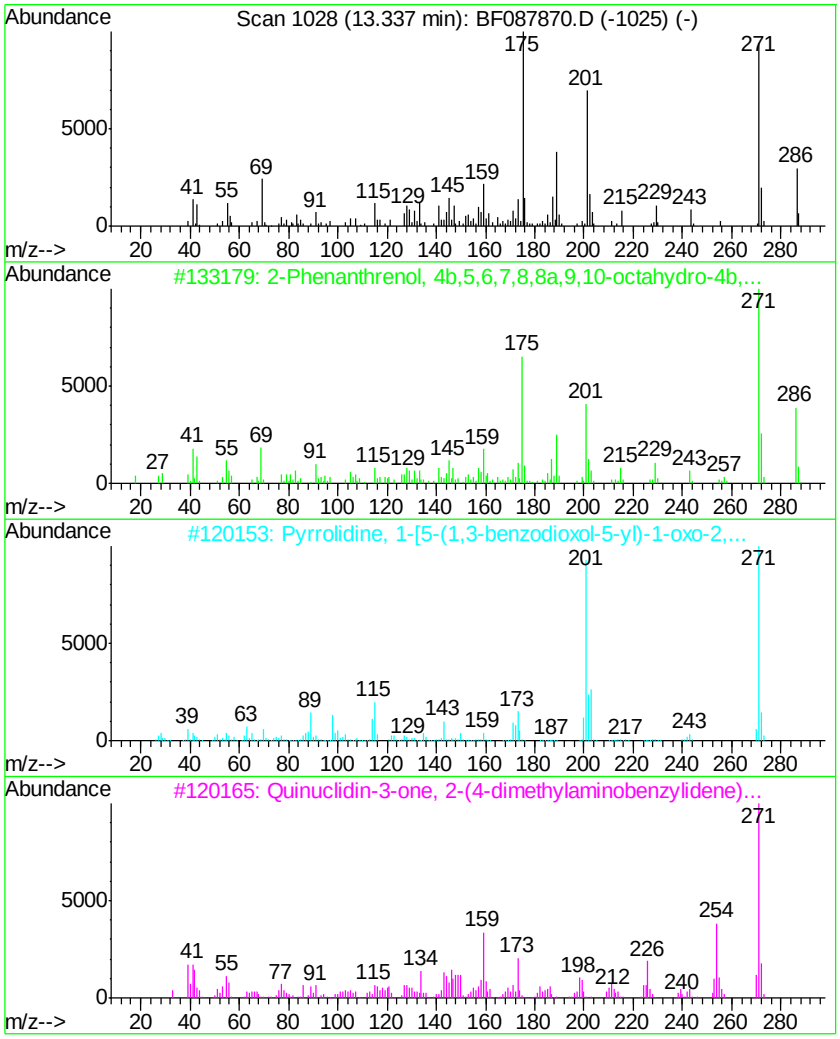
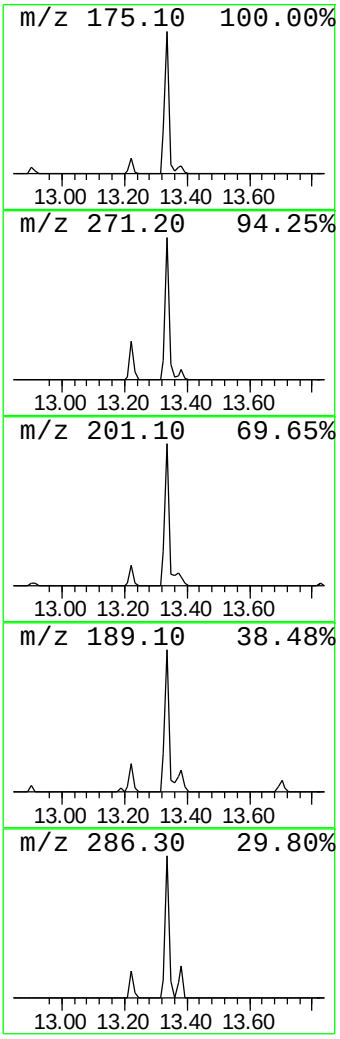
Peak Number 9 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	5.13 ng	250485	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	95
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	30
3	Quinuclidin-3-one, 2-(4-dimethyl...	271	C16H21N3O	1000266-14-6	22
4	Benz(a)acridine, 9,10,12-trimethyl-	271	C20H17N	063040-02-8	18
5	Carbonic acid, monoamide, N-(4-p...	271	C16H17NO3	1000340-19-7	18





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TIC Library : C:\Database\NIST11.L
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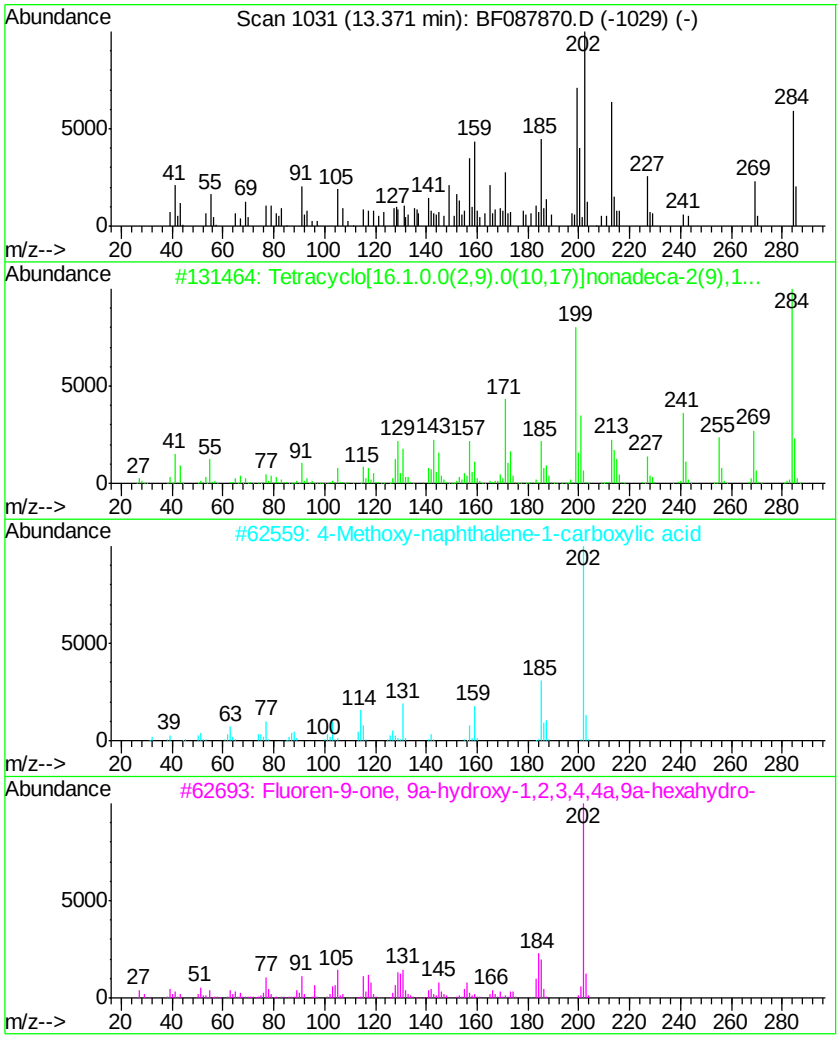
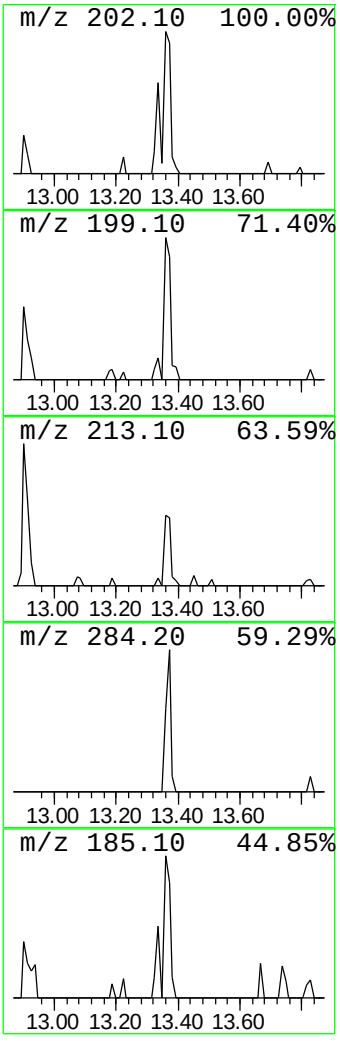
Peak Number 10 unknown13.37 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	3.23 ng	157563	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracyclo[16.1.0.0(2,9).0(10,17...	284	C21H32	1000163-57-5	30
2	4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	25
3	Fluoren-9-one, 9a-hydroxy-1,2,3,...	202	C13H14O2	1000160-37-9	25
4	4-Carbamoyl-3-methoxyquinoline	202	C11H10N2O2	020844-05-7	20
5	1H-Pyrazole-4-carbaldehyde, 5-hy...	202	C11H10N2O2	1000302-68-8	20





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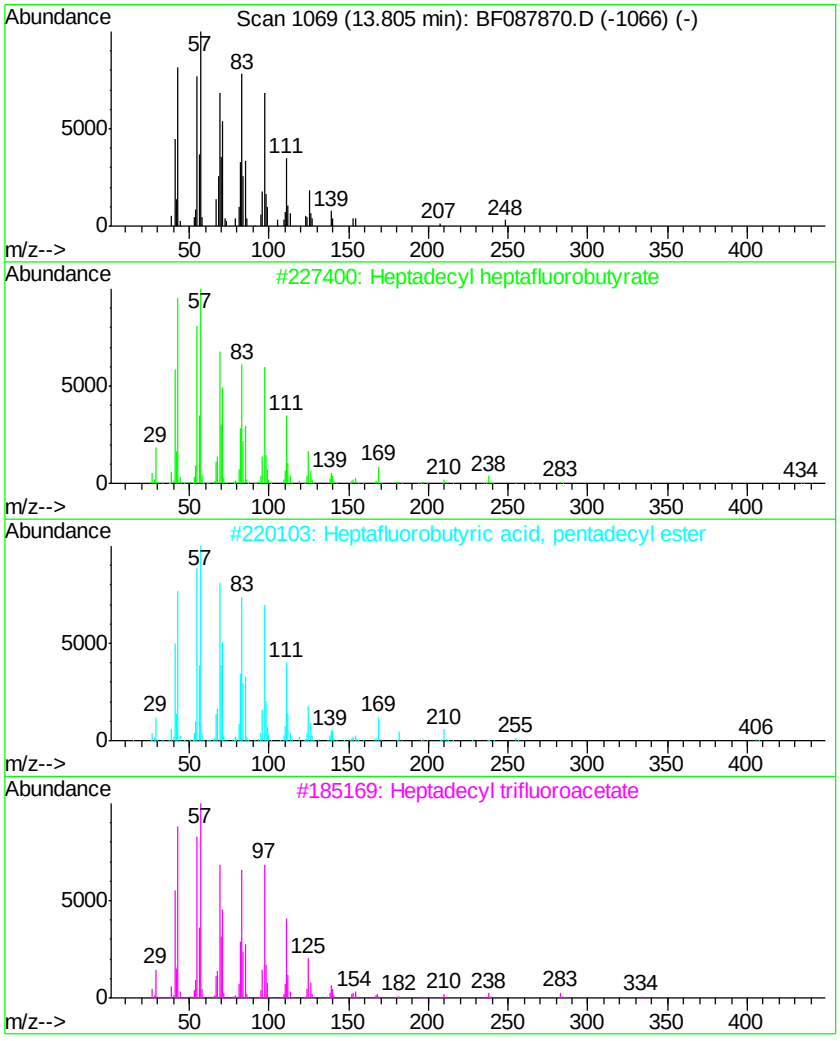
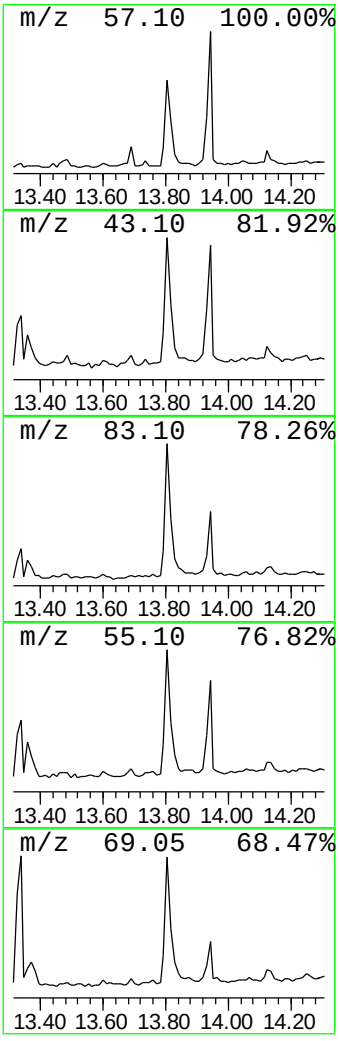
Peak Number 11 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.95 ng	143895	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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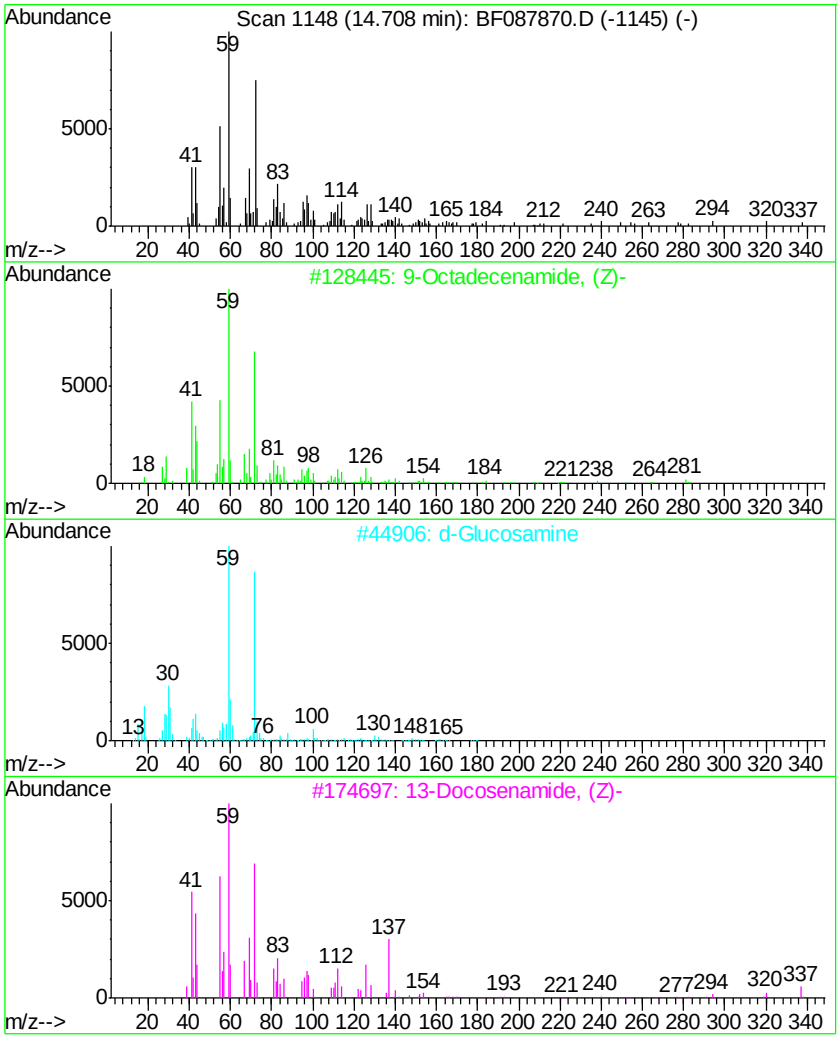
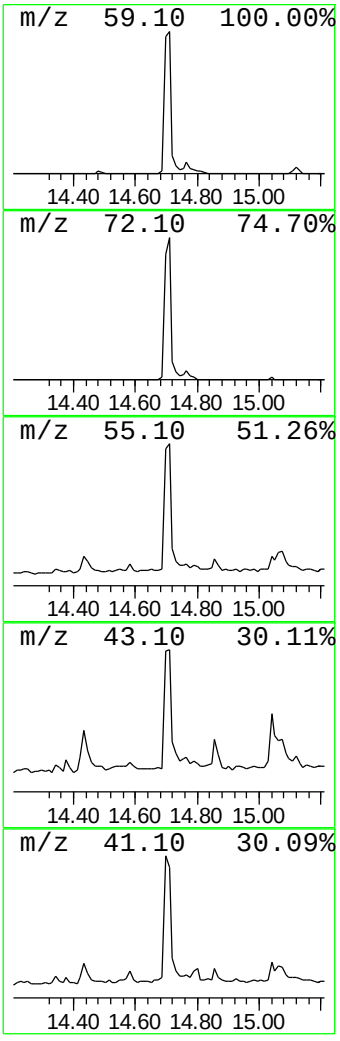
Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	8.38 ng	297094	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	d-Glucosamine	179	C6H13NO5	000090-77-7	50
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	46
4	Decanamide-	171	C10H21NO	002319-29-1	43
5	Tetradecanamide	227	C14H29NO	000638-58-4	38





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Instrument : BNA_F
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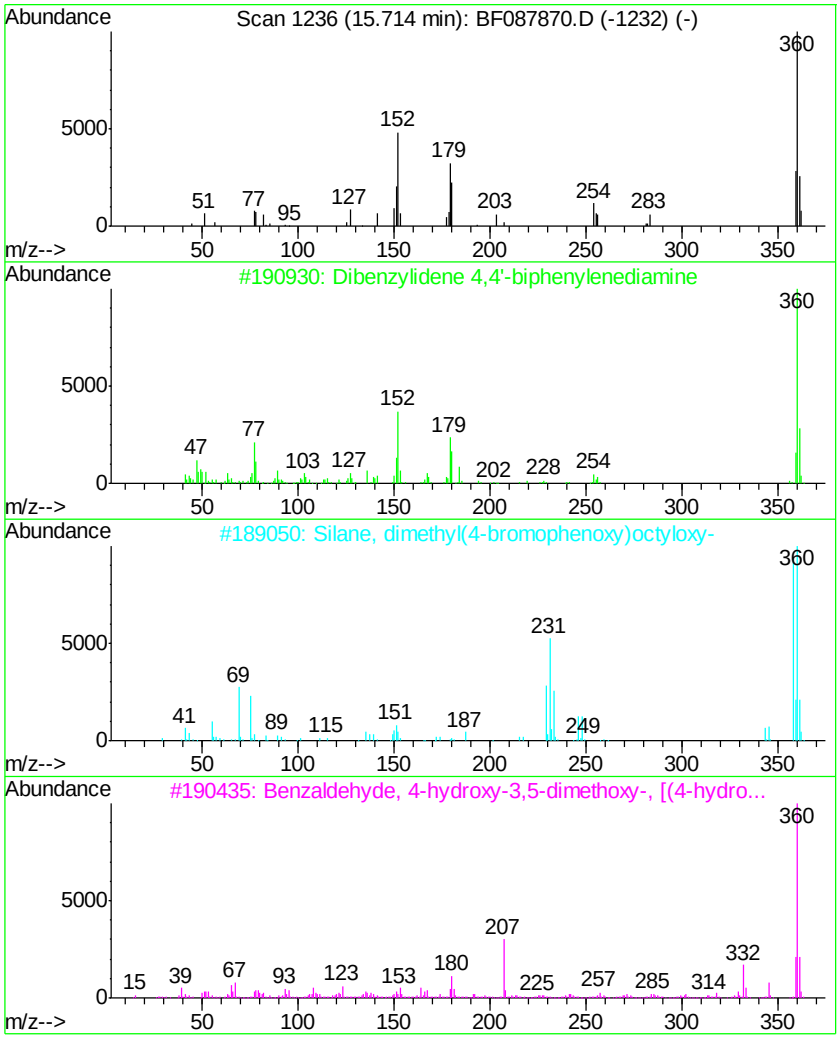
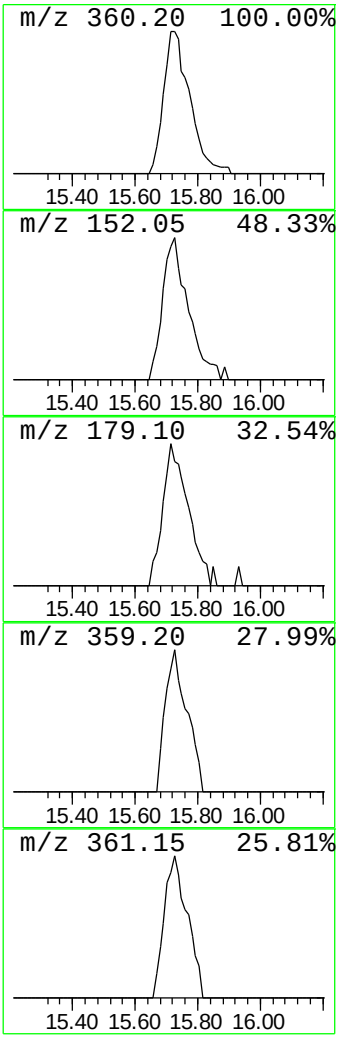
Peak Number 13 Dibenzylidene 4,4'-biphenyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.07 ng	73540	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	87
2	Silane, dimethyl(4-bromophenoxy)...	358	C16H27BrO2Si	1000347-11-2	47
3	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	38
5	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13BO6	1000150-23-7	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087870.D
Acq On : 10 Jun 2016 13:06
Operator : UM/SJ
Sample : H3426-14
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-58

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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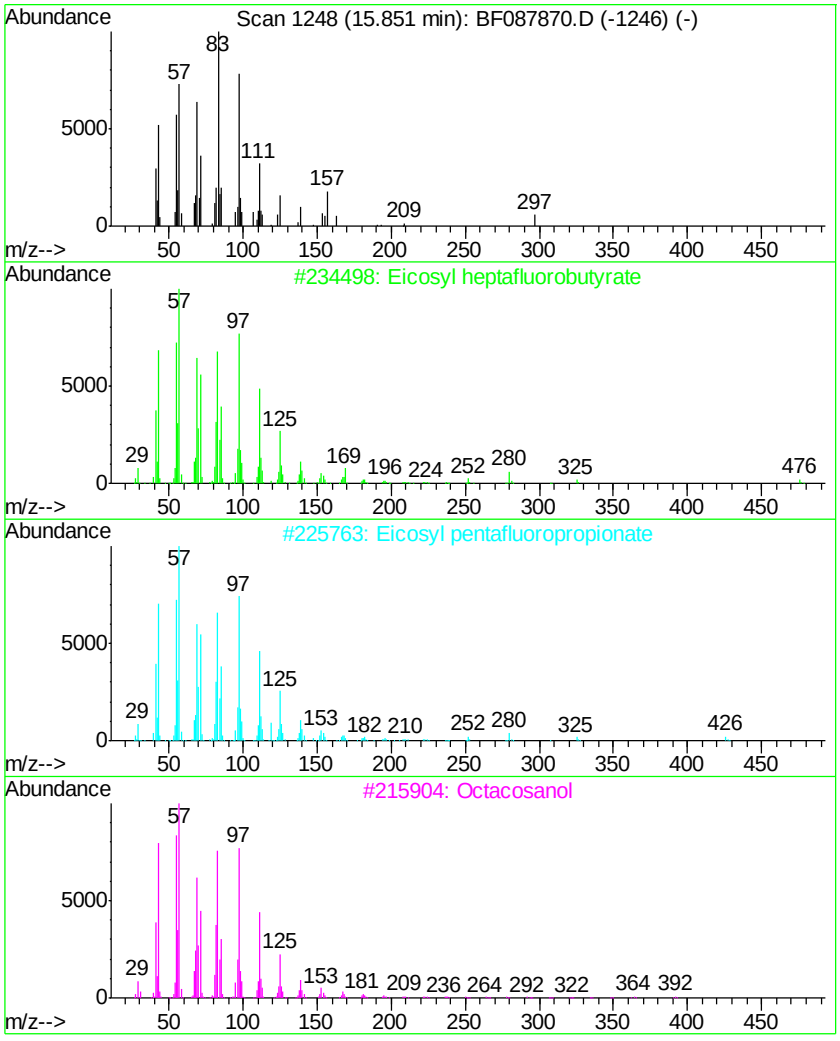
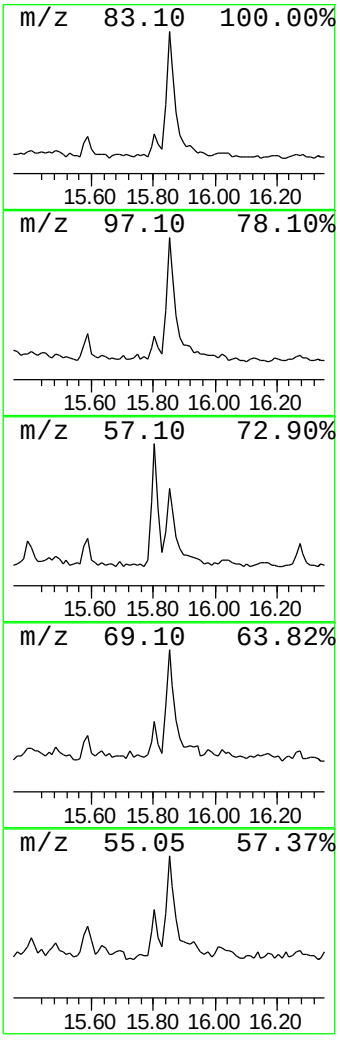
Peak Number 14 Eicosyl heptafluorobutyrate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	2.24 ng	79457	Perylene-d12	15.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	55
2	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	55
3	Octacosanol	410	C28H58O	000557-61-9	53
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	49
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
Data File : BF087870.D
Acq On : 10 Jun 2016 13:06
Operator : UM/SJ
Sample : H3426-14
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SS-58

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.98	4.8	ng	177709	1	6.81	743685	20.0
unknown6.58	6.58	56.2	ng	2089890	1	6.81	743685	20.0
unknown7.46	7.46	2.8	ng	136515	2	8.10	963570	20.0
Dodecanamide	12.42	2.3	ng	132572	4	11.32	1159680	20.0
Butyl citrate	12.73	2.5	ng	122553	5	13.94	976980	20.0
2-Phenanthrenol, ...	13.34	5.1	ng	250485	5	13.94	976980	20.0
unknown13.37	13.37	3.2	ng	157563	5	13.94	976980	20.0
Heptadecyl heptaf...	13.81	3.0	ng	143895	5	13.94	976980	20.0
9-Octadecenamide,...	14.71	8.4	ng	297094	6	15.36	708976	20.0
Dibenzylidene 4,4...	15.71	2.1	ng	73540	6	15.36	708976	20.0
Eicosyl heptafluo...	15.85	2.2	ng	79457	6	15.36	708976	20.0