LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032516\
Data File : BF085781.D
Acq On : 26 Mar 2016 00:35
Operator : UM/SJ
Sample : H1834-08
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 13

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-BF032416.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	5.007	235	238	244	rBV	301951	483191	15.75%	1.898%
2	5.430	272	275	277	rBV	2268292	2827158	92.13%	11.105%
3	5.830	307	310	312	rVB	45383	48820	1.59%	0.192%
4	6.459	362	365	368	rBV	1865817	2795363	91.09%	10.980%
5	6.596	374	377	379	rBV	2809373	2901326	94.54%	11.396%
6	6.824	395	397	399	rBV	739008	625925	20.40%	2.459%
7	6.984	408	411	413	rBV	2228657	2374460	77.37%	9.326%
8	7.396	444	447	449	rBV	1588106	1936317	63.10%	7.606%
9	7.499	453	456	462	rVB	48852	74295	2.42%	0.292%
10	8.104	507	509	512	rBV	646439	756822	24.66%	2.973%
11	9.190	601	604	606	rBV	2927628	3068781	100.00%	12.054%
12	9.579	636	638	640	rBV	593264	509084	16.59%	2.000%
13	9.796	656	657	659	rVB	64362	46085	1.50%	0.181%
14	9.865	661	663	665	rVB	699850	682914	22.25%	2.682%
15	10.299	697	701	702	rBV2	55426	86662	2.82%	0.340%
16	10.516	717	720	721	rBV	43280	57846	1.88%	0.227%
17	10.653	729	732	734	rBV	1459720	1503291	48.99%	5.905%
18	10.768	740	742	747	rVB	83785	128713	4.19%	0.506%
19	11.213	779	781	782	rBV	43592	36911	1.20%	0.145%
20	11.248	782	784	787	rVB	33042	44578	1.45%	0.175%
21	11.339	790	792	795	rBV2	481057	567063	18.48%	2.227%
22	11.876	837	839	843	rBV	78591	97495	3.18%	0.383%
23	12.653	905	907	913	rBV4	19231	33740	1.10%	0.133%
24	12.745	913	915	918	rVB	132725	142990	4.66%	0.562%
25	12.928	928	931	933	rBV	2315754	2111375	68.80%	8.293%
26	13.408	970	973	975	rBV	241651	230914	7.52%	0.907%
27	13.454	975	977	979	rVB	40467	35289	1.15%	0.139%
28	13.774	1003	1005	1007	rVB	94859	79894	2.60%	0.314%
29	13.831	1007	1010	1016	rVB	63705	105412	3.43%	0.414%
30	13.979	1020	1023	1025	rBV	607279	587944	19.16%	2.309%
31	15.397	1144	1147	1150	rBV	412915	478738	15.60%	1.880%

Sum of corrected areas: 25459396

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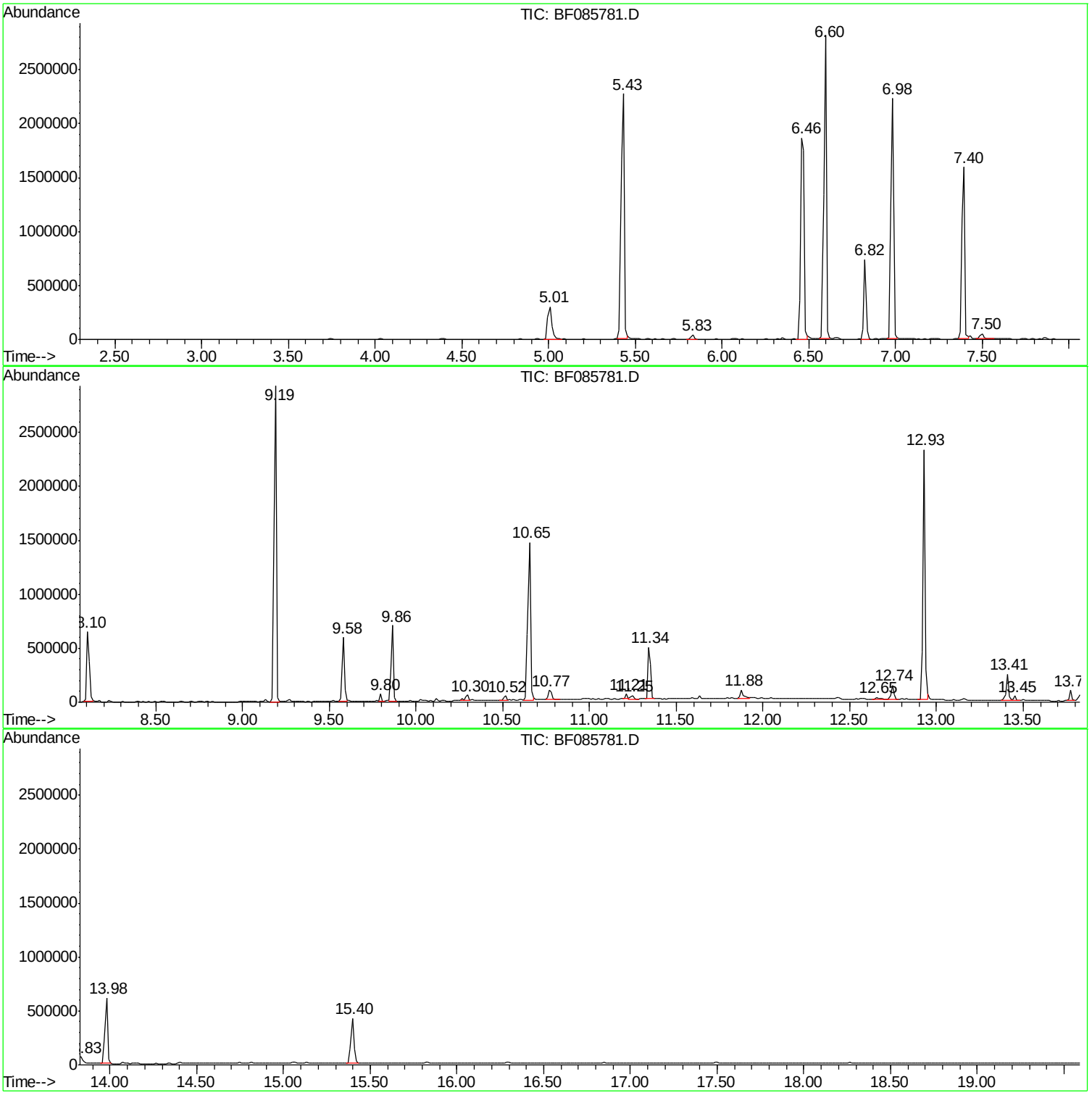
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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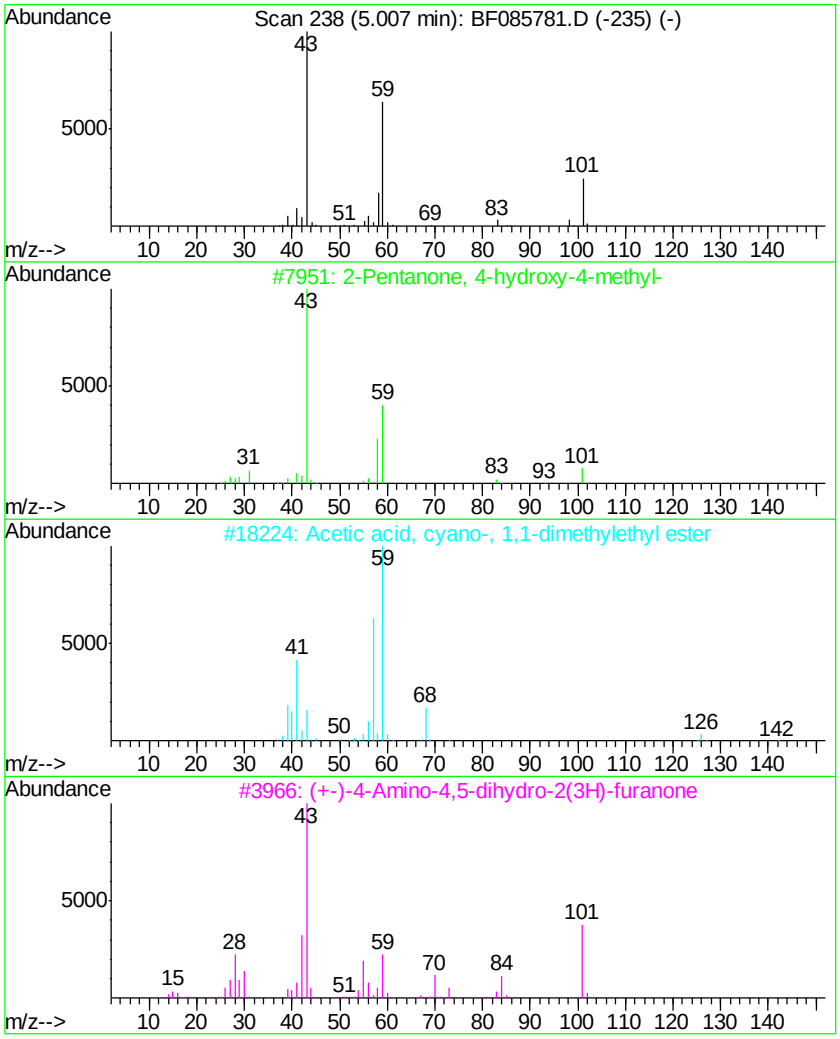
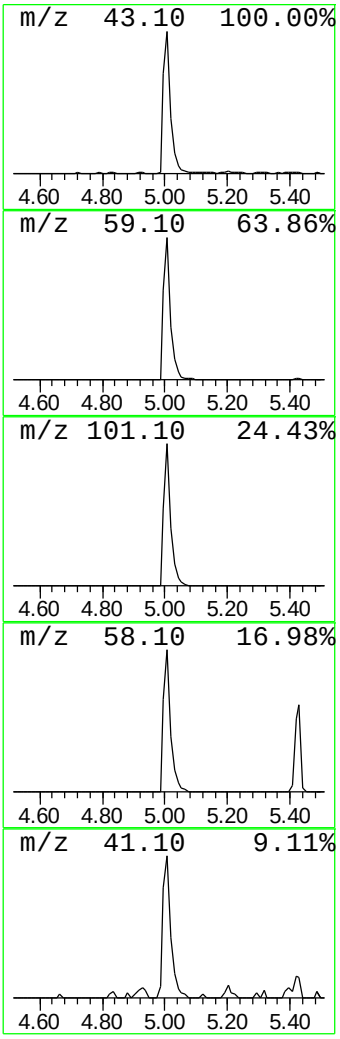
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	15.44 ng	483191	1,4-Dichlorobenzene-d4	6.82

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	23
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Sample : H1834-08
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Instrument : BNA_F
ClientSampleId : 13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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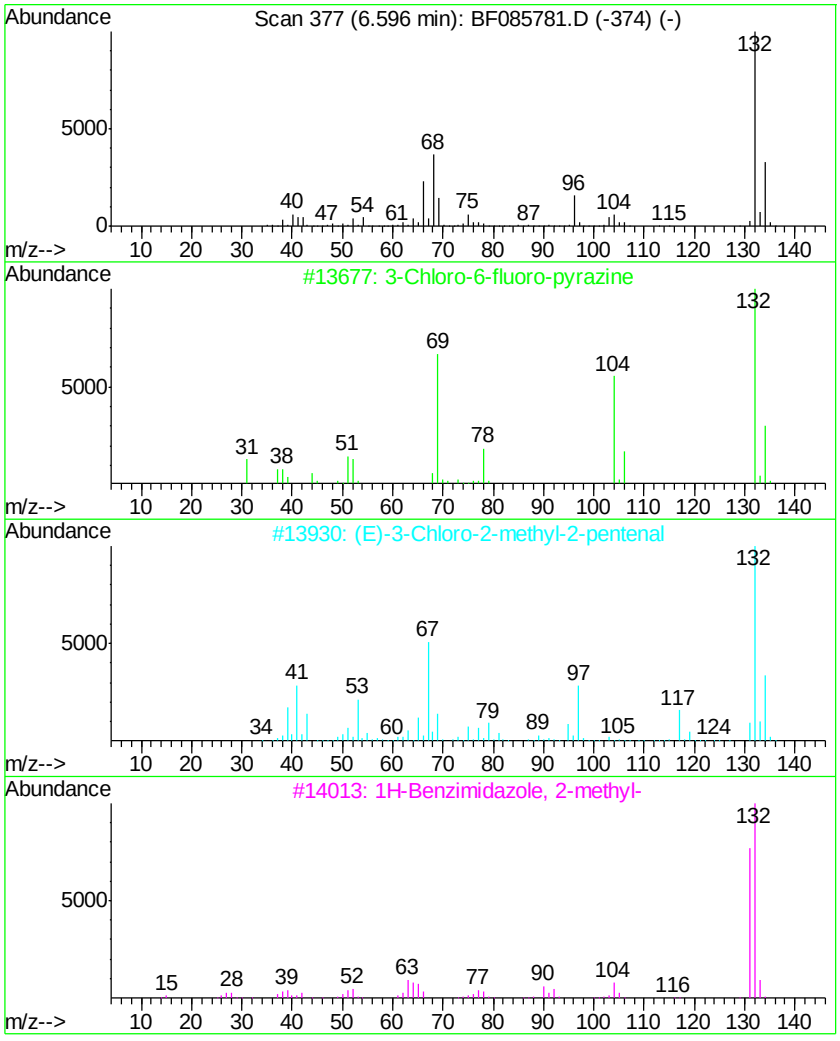
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

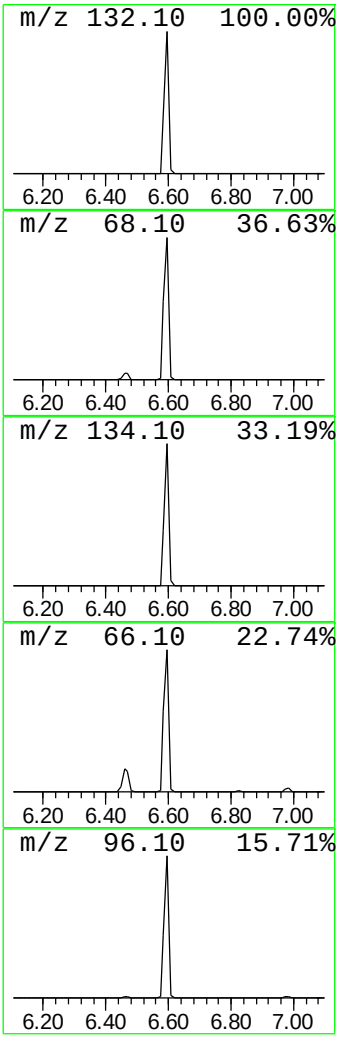
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	92.71 ng	2901330	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032516\
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Misc :
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Instrument : BNA_F
ClientSampleId : 13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

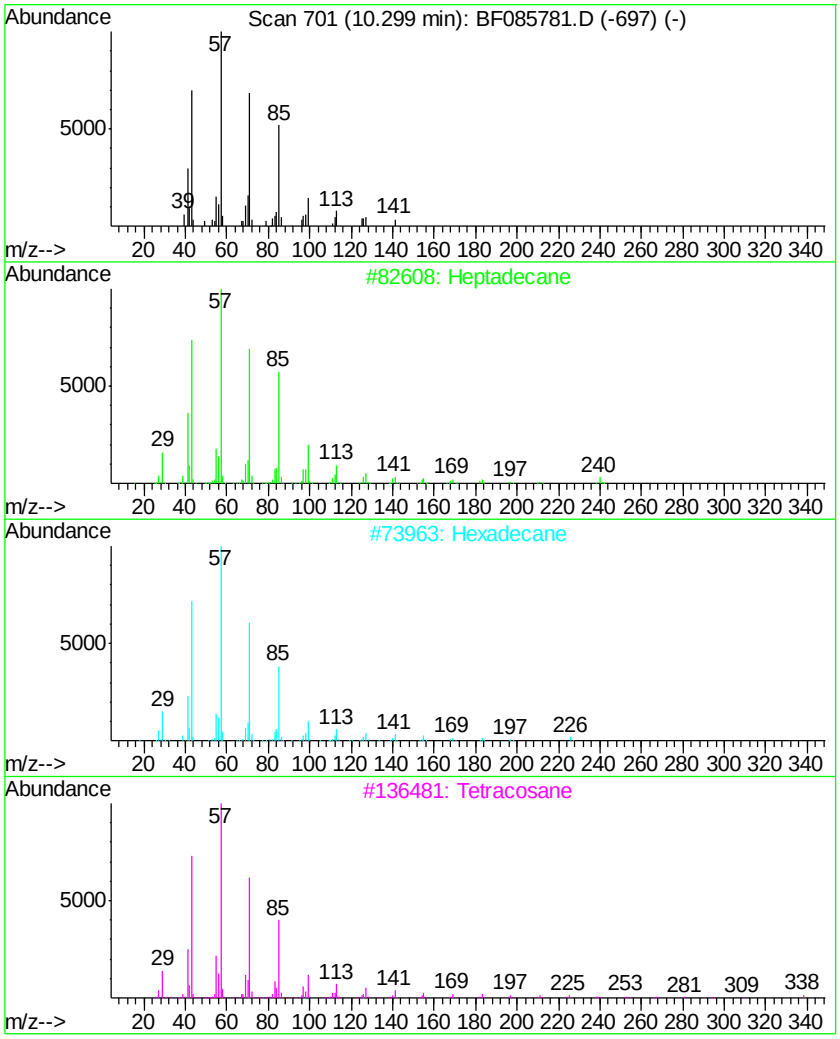
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

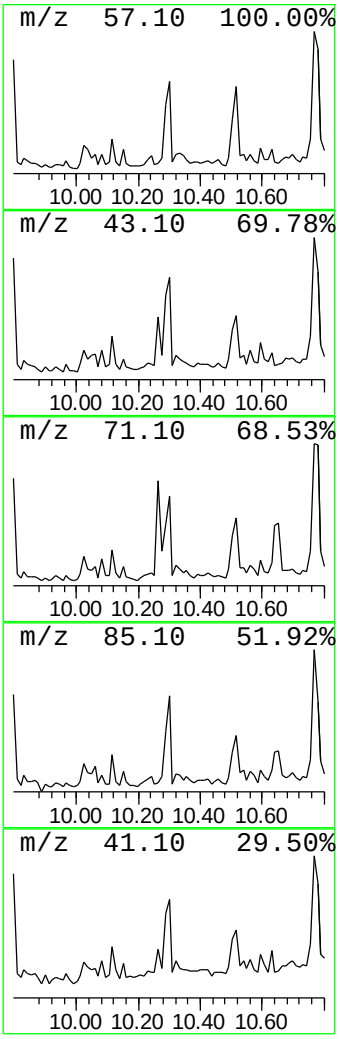
****

Peak Number 4 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	2.54 ng	86662	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetracosane	338	C24H50	000646-31-1	87
4	Octadecane	254	C18H38	000593-45-3	86
5	Tetradecane	198	C14H30	000629-59-4	86





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Sample : H1834-08
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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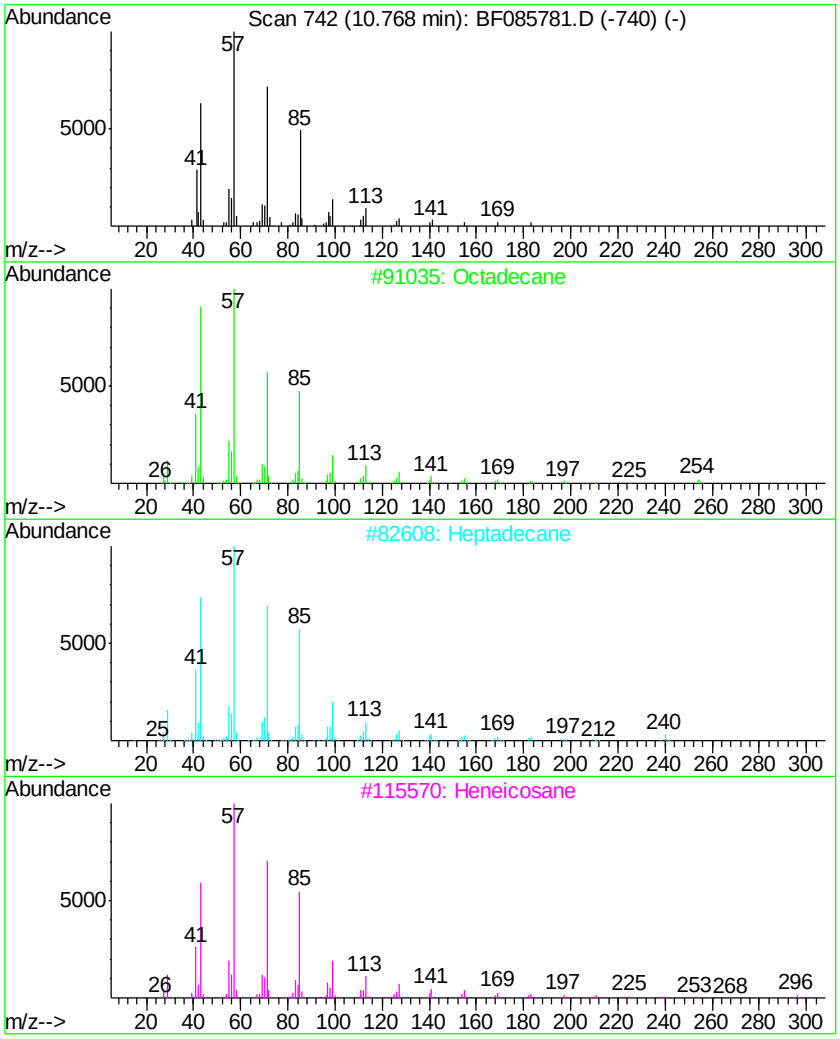
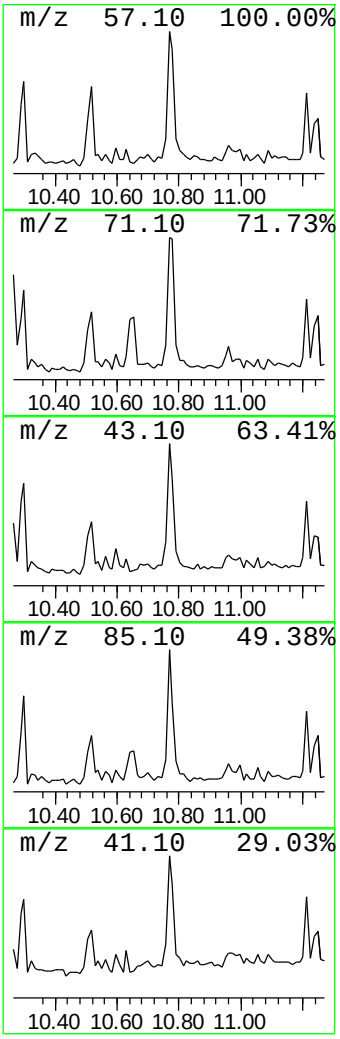
Peak Number 5 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	4.54 ng	128713	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Pentadecane	212	C15H32	000629-62-9	87





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Sample : H1834-08
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Instrument : BNA_F
ClientSampleId : 13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Library : C:\DATABASE\NIST02.L
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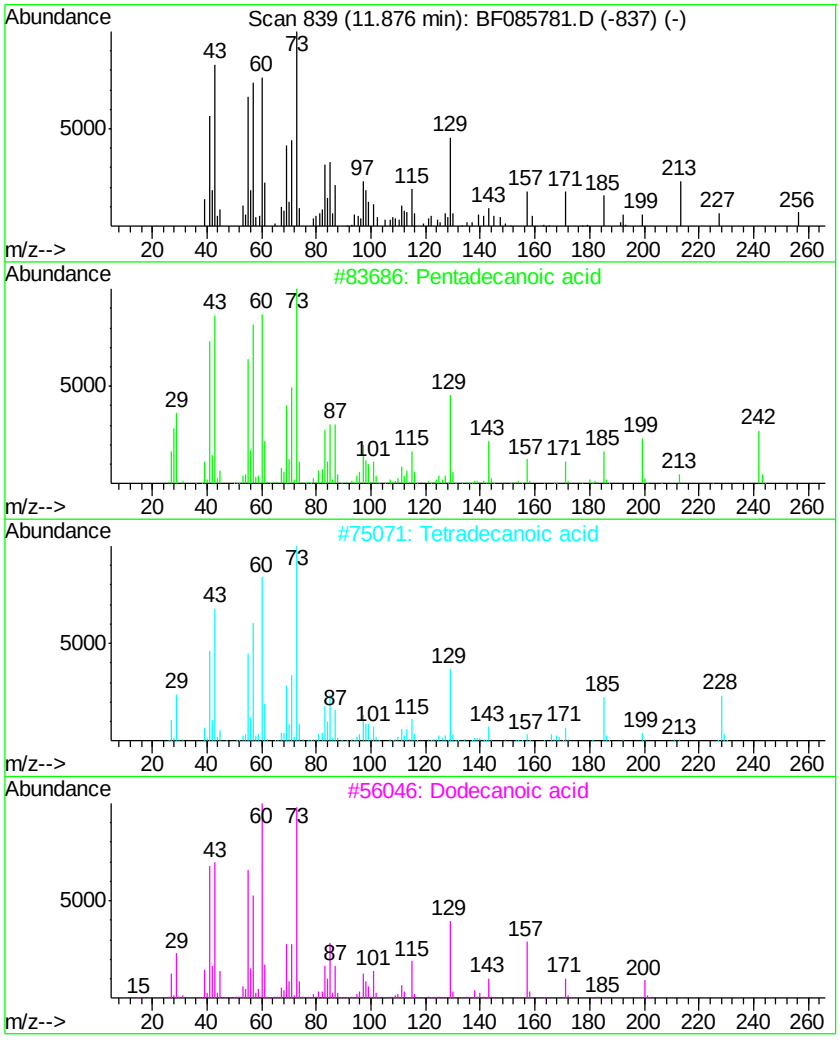
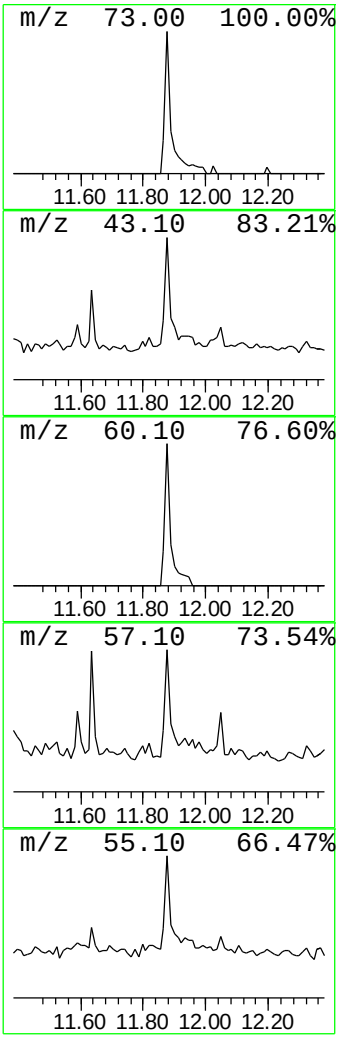
Peak Number 6 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	3.44 ng	97495	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Dodecanoic acid	200	C12H24O2	000143-07-7	50
4	d-Glucitol, 4-O-octyl-	294	C14H30O6	132696-01-6	14
5	.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	14





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Instrument : BNA_F
ClientSampleId : 13

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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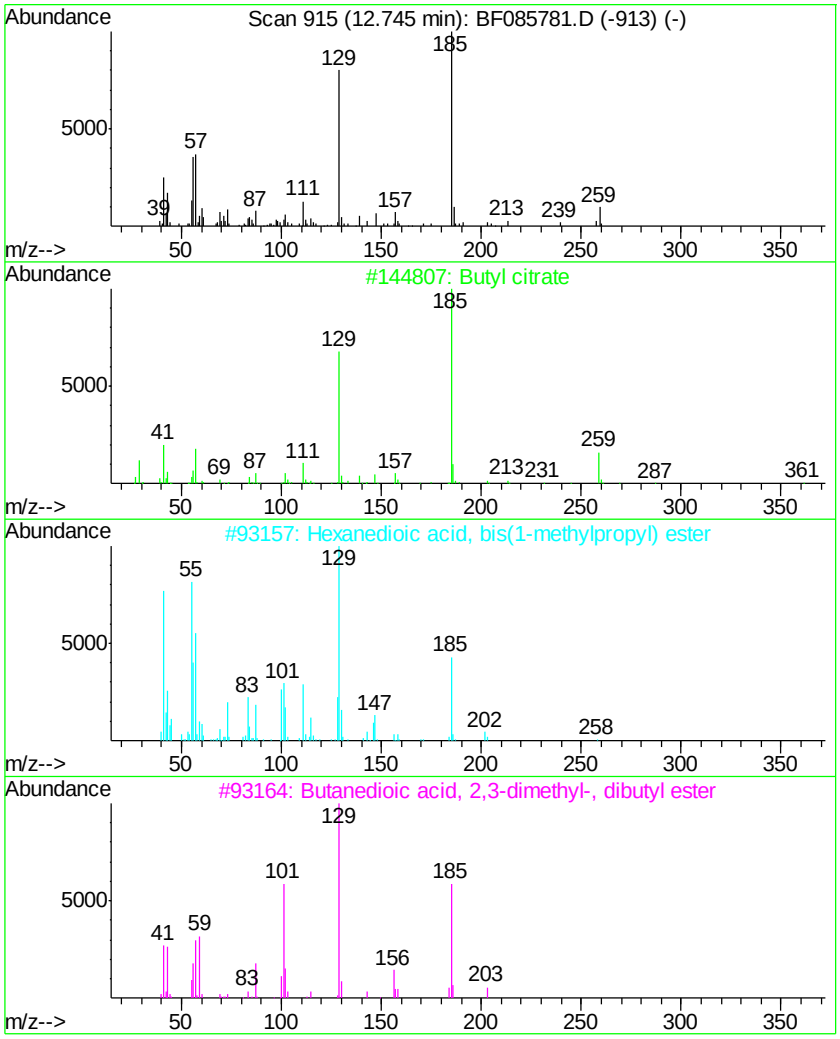
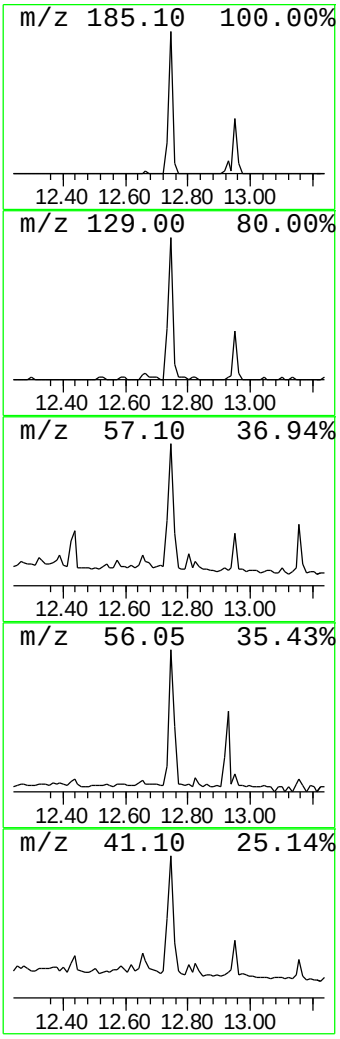
Peak Number 7 Butyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	4.86 ng	142990	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	74
2	Hexanedioic acid, bis(1-methylpr...	258	C14H26O4	038447-22-2	50
3	Butanedioic acid, 2,3-dimethyl-,...	258	C14H26O4	056051-57-1	45
4	Hexanedioic acid, dibutyl ester	258	C14H26O4	000105-99-7	42
5	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	37





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Instrument : BNA_F
ClientSampleId : 13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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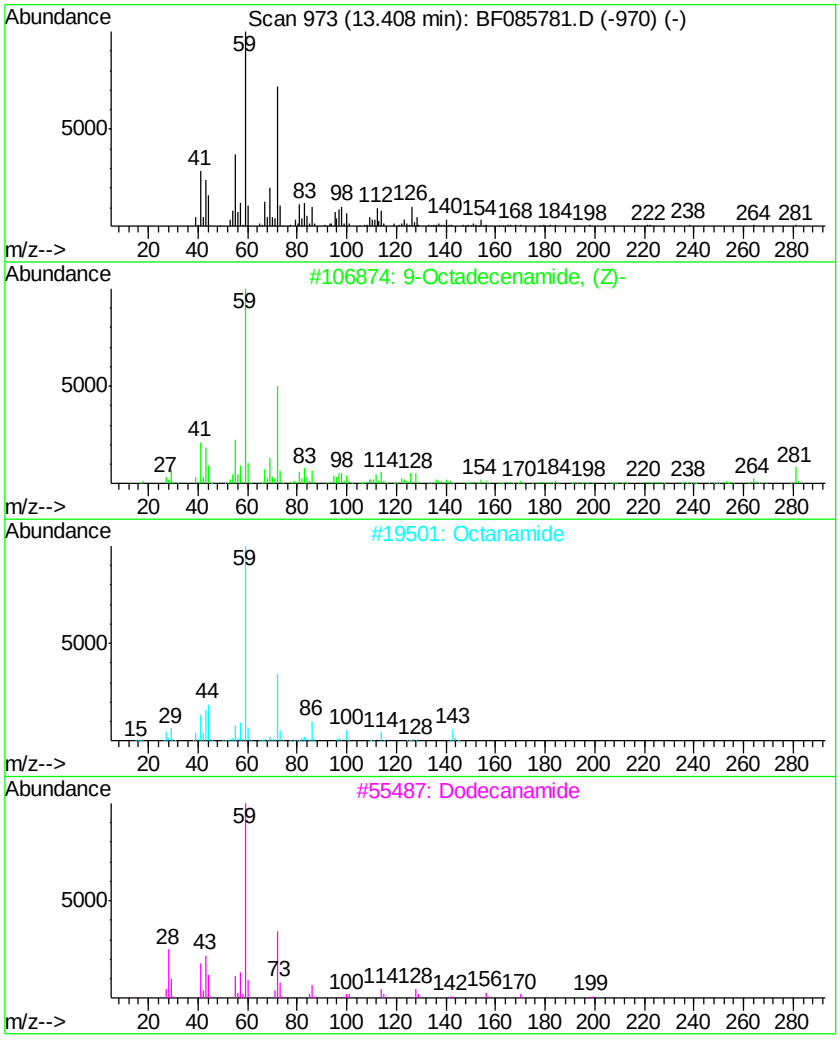
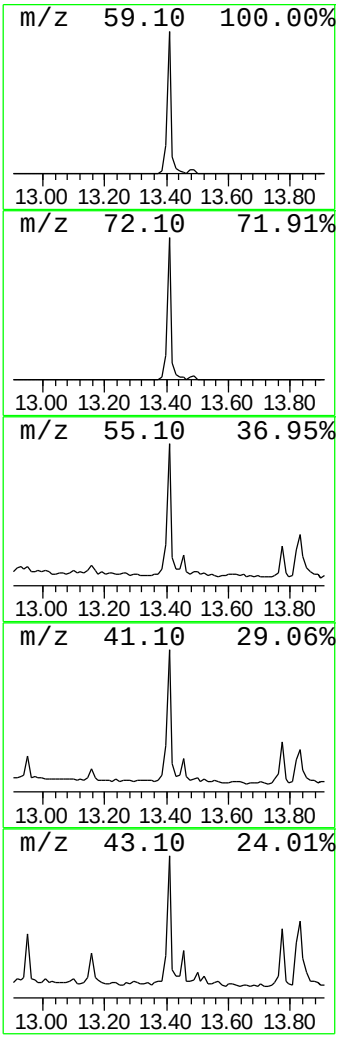
Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	7.85 ng	230914	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Octanamide	143	C8H17NO	000629-01-6	53
3	Dodecanamide	199	C12H25NO	001120-16-7	53
4	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43
5	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	38





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TIC Library : C:\DATABASE\NIST02.L
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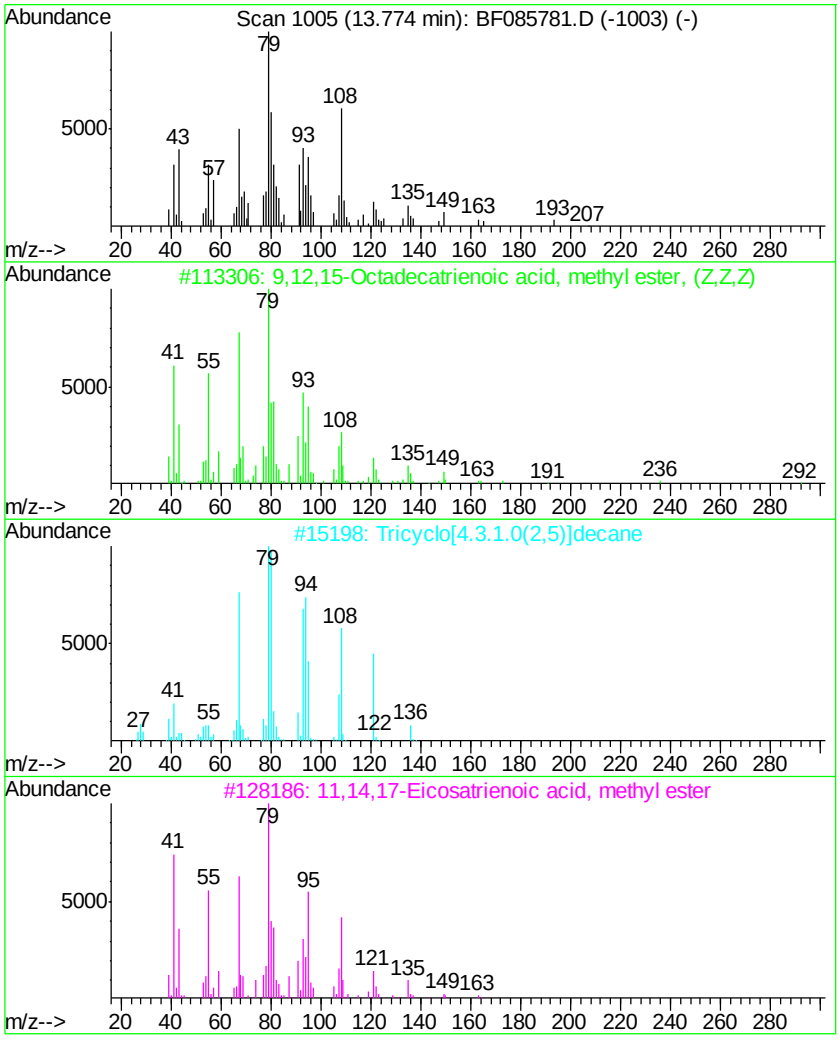
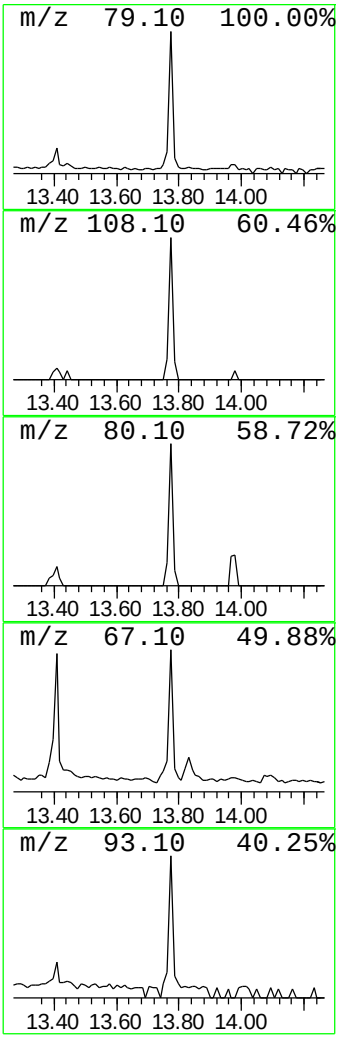
Peak Number 9 9,12,15-Octadecatrienoic ac... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.72 ng	79894	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12,15-Octadecatrienoic acid, m...	292	C19H32O2	000301-00-8	52
2	Tricyclo[4.3.1.0(2,5)]decane	136	C10H16	042210-02-6	52
3	11,14,17-Eicosatrienoic acid, me...	320	C21H36O2	055682-88-7	50
4	17-Octadecen-14-yn-1-ol	264	C18H32O	018202-28-3	50
5	cis,cis,cis-7,10,13-Hexadecatrienal	234	C16H26O	056797-43-4	49





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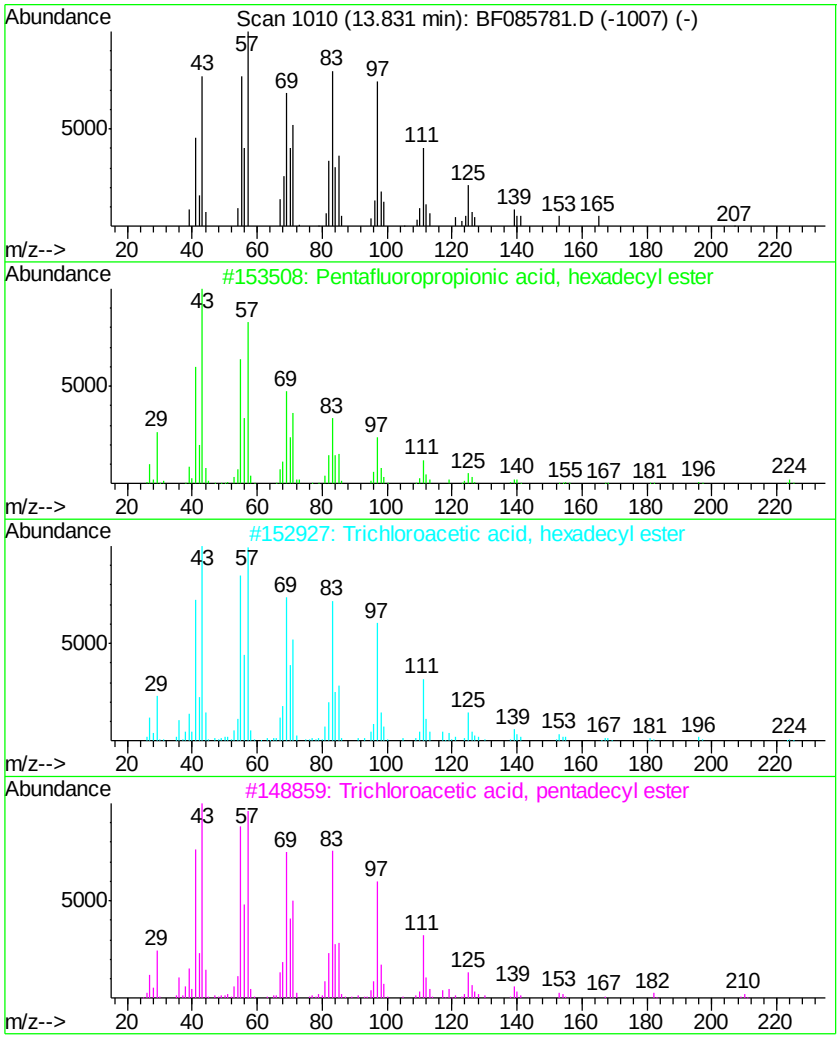
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

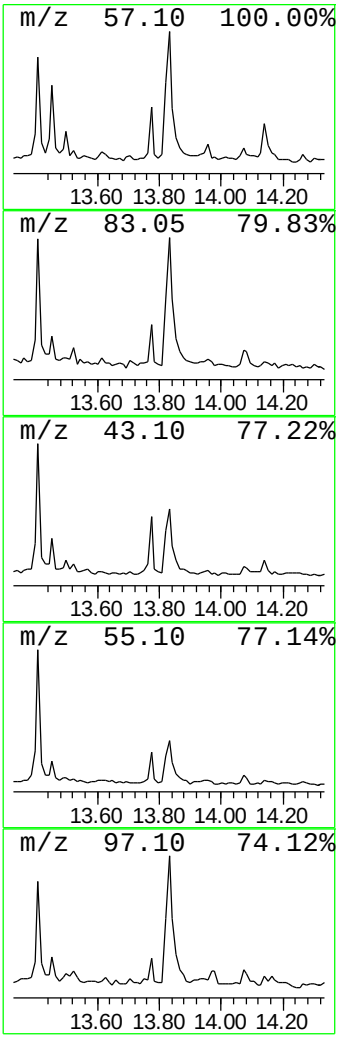
****

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.59 ng	105412	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	90
5	1-Nonadecene	266	C19H38	018435-45-5	90





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	15.4	ng	483191	1	6.82	625925	20.0
unknown6.60	6.60	92.7	ng	2901330	1	6.82	625925	20.0
Heptadecane	10.30	2.5	ng	86662	3	9.86	682914	20.0
Octadecane	10.77	4.5	ng	128713	4	11.34	567063	20.0
Pentadecanoic acid	11.88	3.4	ng	97495	4	11.34	567063	20.0
Butyl citrate	12.74	4.9	ng	142990	5	13.98	587944	20.0
9-Octadecenamide,...	13.41	7.8	ng	230914	5	13.98	587944	20.0
9,12,15-Octadecat...	13.77	2.7	ng	79894	5	13.98	587944	20.0
Pentafluoropropio...	13.83	3.6	ng	105412	5	13.98	587944	20.0