LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085756.D
Acq On : 25 Mar 2016 11:48
Operator : UM/SJ
Sample : H1858-03
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-13A

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	248	rBV	697525	1071197	30.56%	3.710%
2	5.430	272	275	278	rBV	2811256	3035183	86.58%	10.511%
3	5.830	308	310	320	rVB	104747	110234	3.14%	0.382%
4	6.470	363	366	368	rBV	2772386	3328076	94.94%	11.525%
5	6.596	374	377	379	rBV	3186570	3125866	89.17%	10.825%
6	6.825	395	397	399	rBV	831079	692768	19.76%	2.399%
7	6.985	408	411	413	rBV	2905296	2756021	78.62%	9.544%
8	7.396	444	447	449	rBV	2201211	2309377	65.88%	7.998%
9	8.105	507	509	512	rBV	606512	812039	23.16%	2.812%
10	9.191	601	604	606	rBV	3782093	3505541	100.00%	12.140%
11	9.579	636	638	641	rBV	449476	392585	11.20%	1.360%
12	9.796	655	657	659	rBV	103009	81278	2.32%	0.281%
13	9.865	661	663	665	rVB	856754	770905	21.99%	2.670%
14	10.025	674	677	681	rBV	16654	41697	1.19%	0.144%
15	10.299	697	701	702	rBV	104125	116825	3.33%	0.405%
16	10.516	717	720	723	rBV	37077	58249	1.66%	0.202%
17	10.654	729	732	734	rBV	1728185	1681239	47.96%	5.822%
18	10.768	740	742	747	rVB	117626	127547	3.64%	0.442%
19	11.214	779	781	783	rBV	44880	40816	1.16%	0.141%
20	11.339	790	792	795	rBV2	504454	612192	17.46%	2.120%
21	11.877	836	839	841	rBV	56066	62151	1.77%	0.215%
22	12.928	928	931	934	rBV	2748243	2555073	72.89%	8.848%
23	13.831	1007	1010	1016	rBV	113194	205422	5.86%	0.711%
24	13.980	1020	1023	1025	rBV	708580	680117	19.40%	2.355%
25	14.723	1086	1088	1093	rVB2	64270	97613	2.78%	0.338%
26	15.397	1144	1147	1153	rBV	463480	605878	17.28%	2.098%

Sum of corrected areas: 28875889

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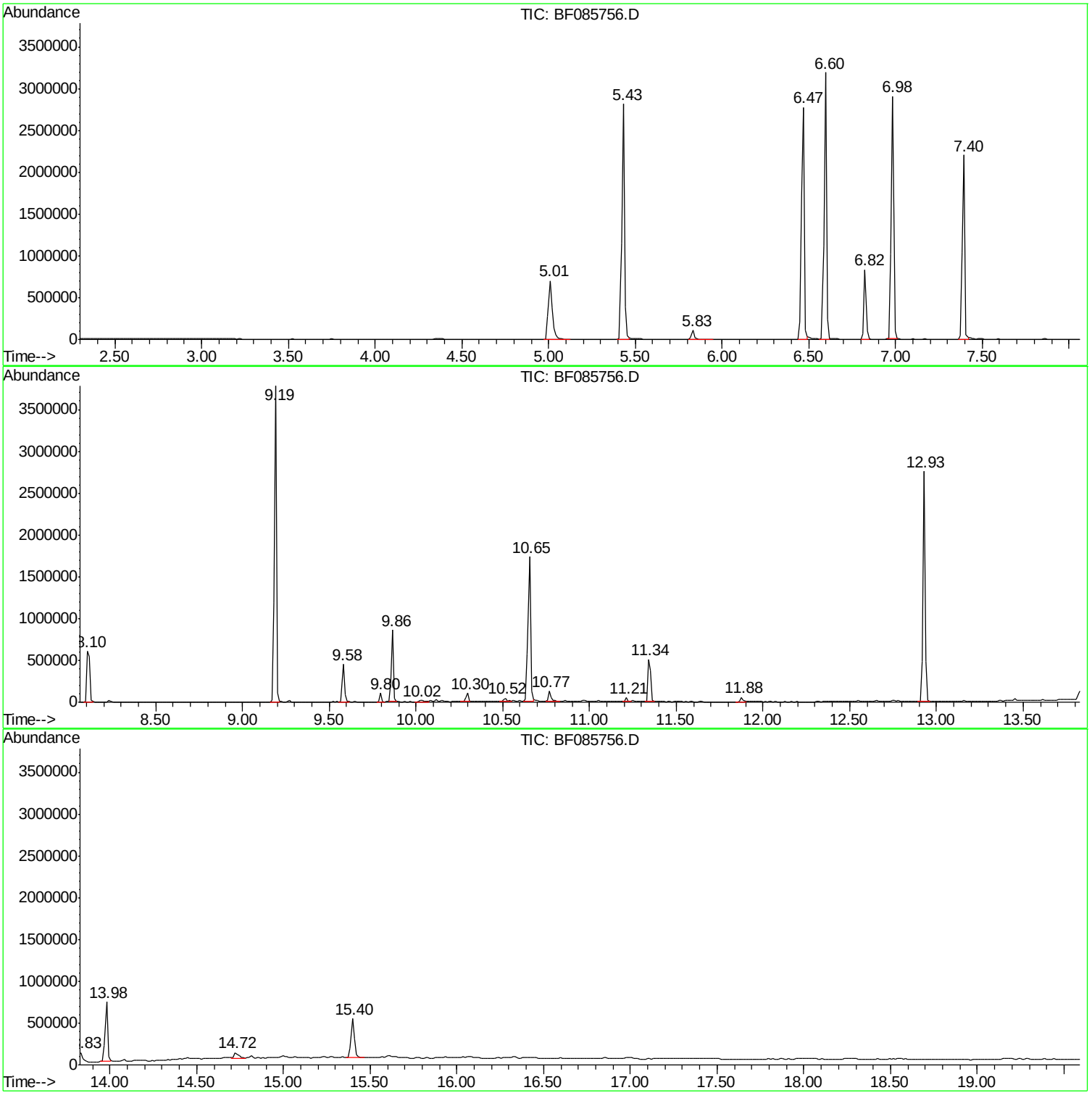
Instrument :
BNA_F
ClientSampleId :
TRACK-D-GRID-13A

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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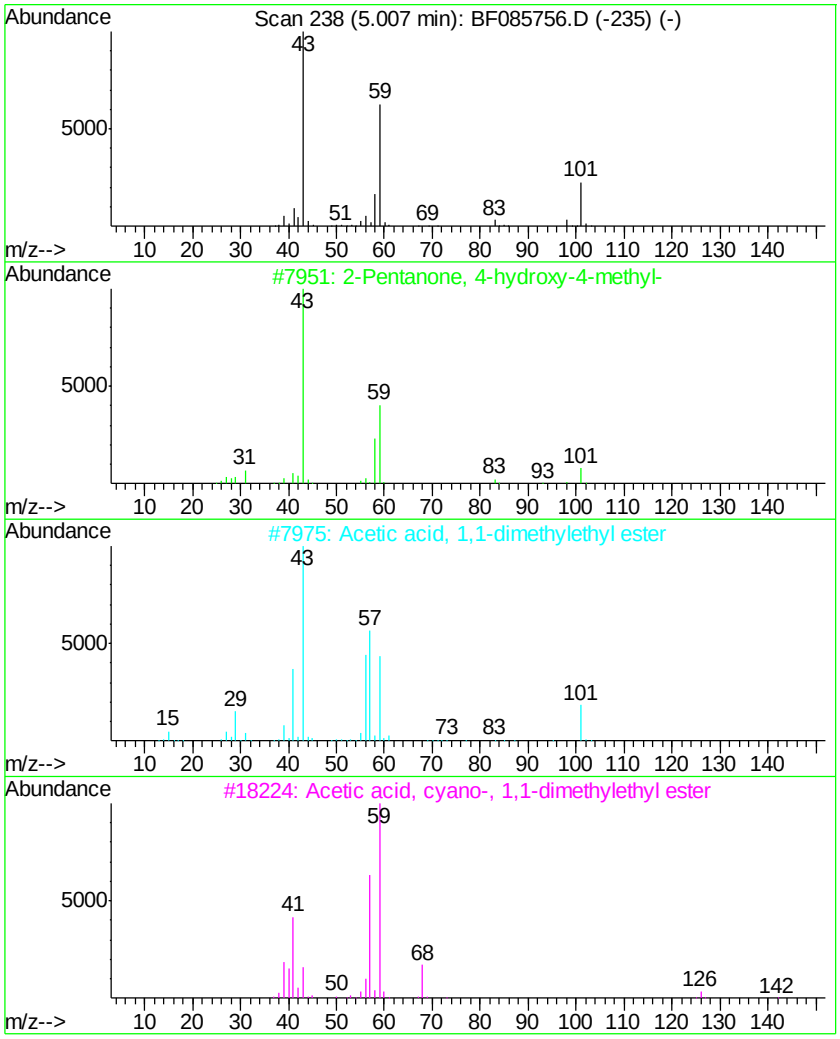
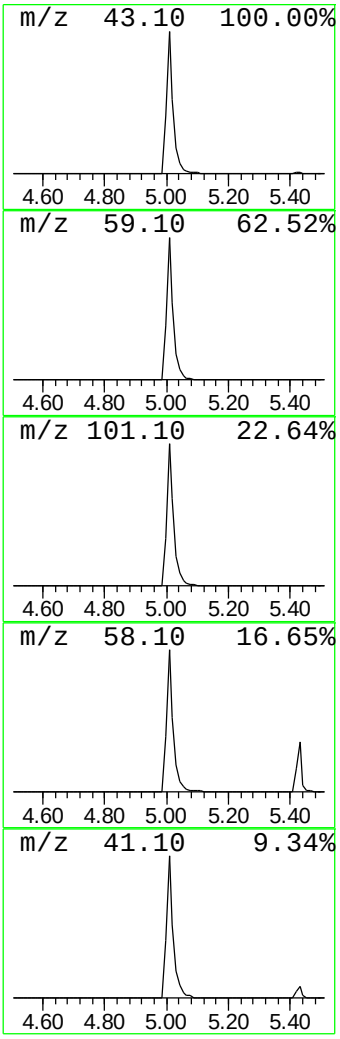
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	30.93 ng	1071200	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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032416\
Data File : BF085756.D
Acq On : 25 Mar 2016 11:48
Operator : UM/SJ
Sample : H1858-03
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-13A

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

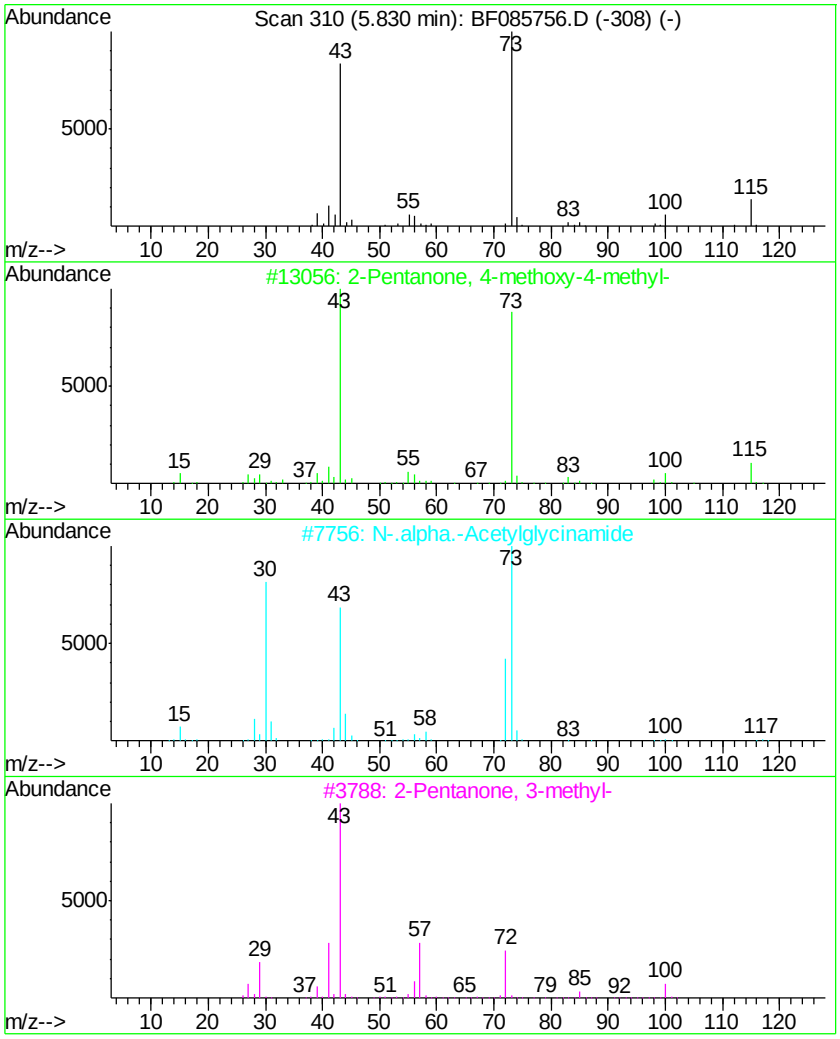
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

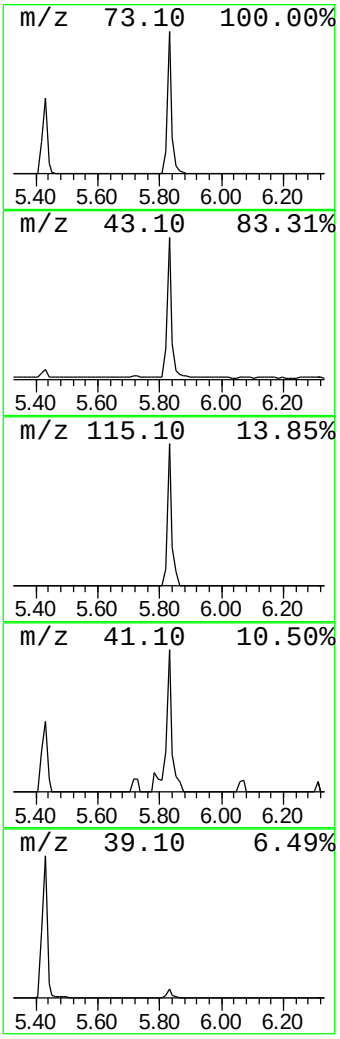
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.83	3.18 ng	110234	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	33
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	27
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12





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Operator : UM/SJ
Sample : H1858-03
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-13A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Library : C:\DATABASE\NIST02.L
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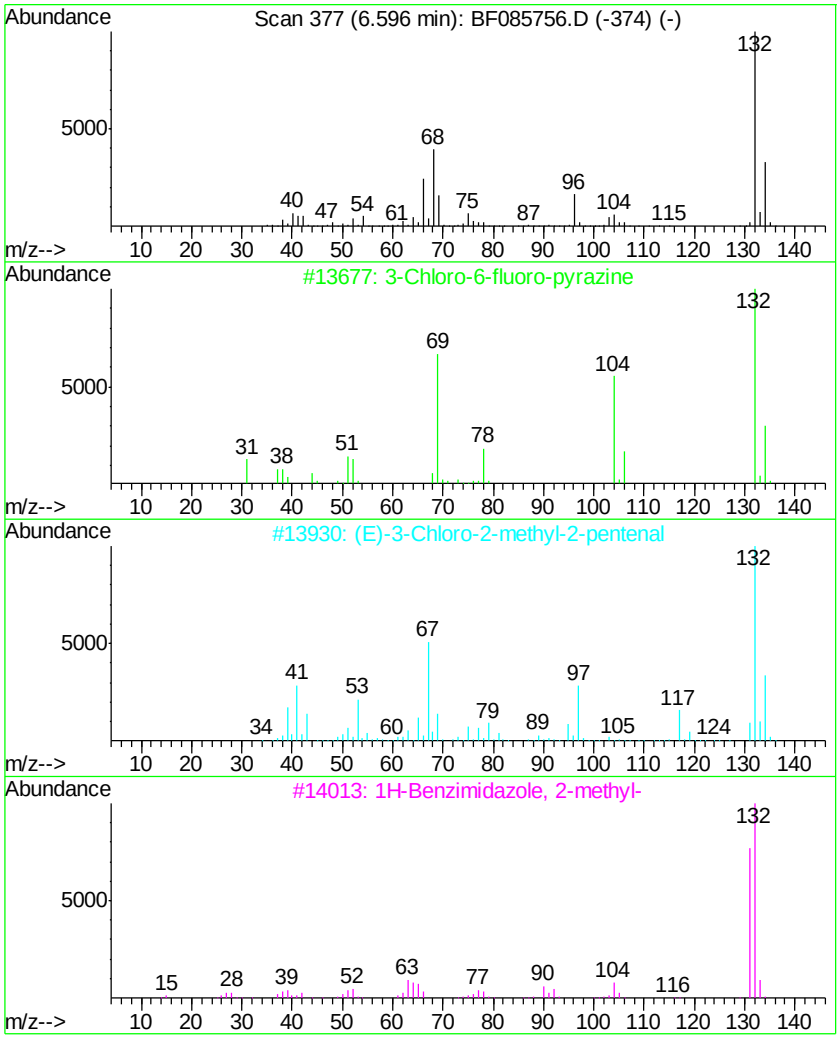
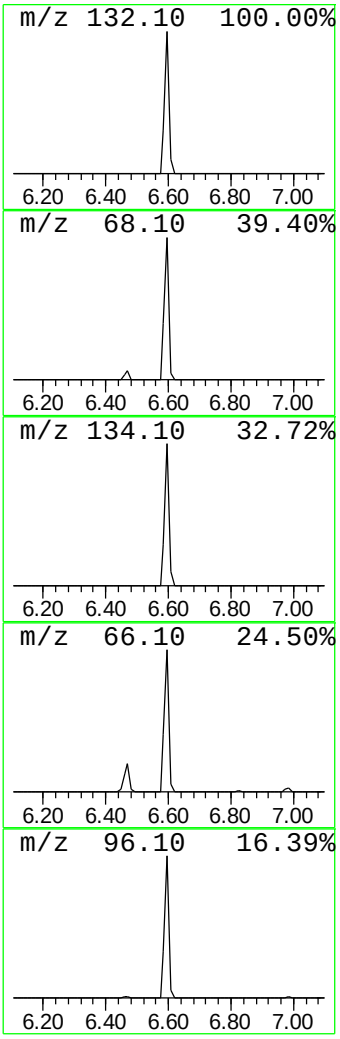
Peak Number 3 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	90.24 ng	3125870	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : H1858-03
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Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-13A

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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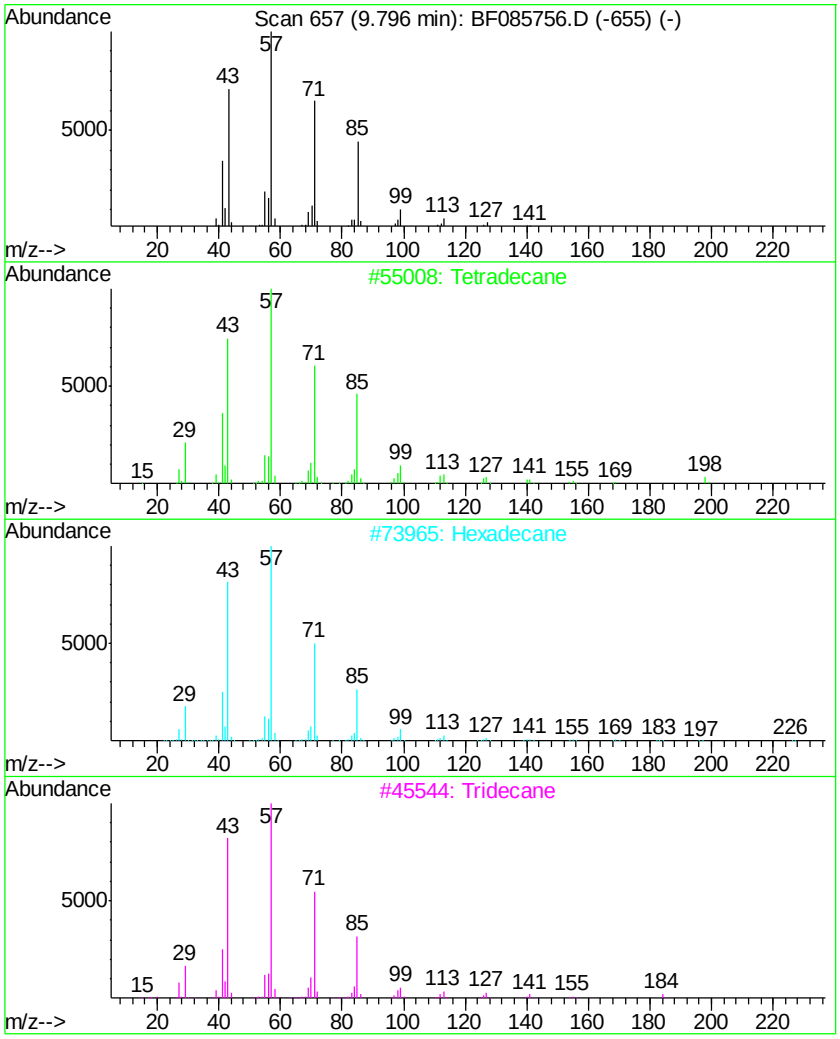
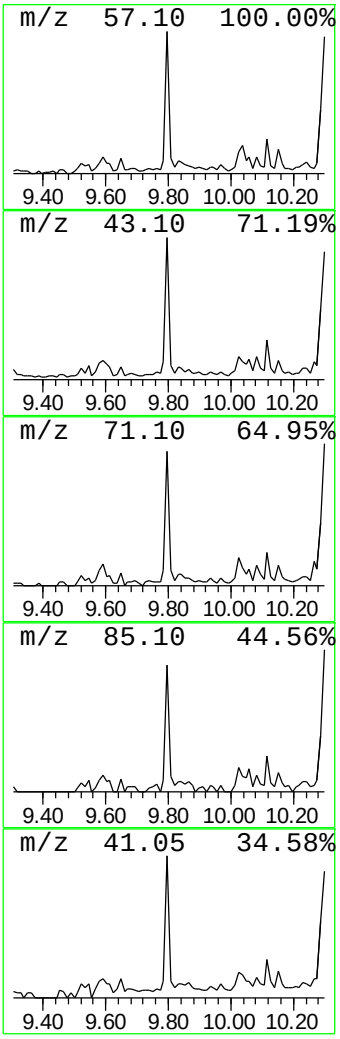
Peak Number 5 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.80	2.11 ng	81278	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Hexadecane	226	C16H34	000544-76-3	80
3	Tridecane	184	C13H28	000629-50-5	72
4	Nonane, 5-butyl-	184	C13H28	017312-63-9	64
5	Pentadecane	212	C15H32	000629-62-9	64





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Data File : BF085756.D
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Operator : UM/SJ
Sample : H1858-03
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-13A

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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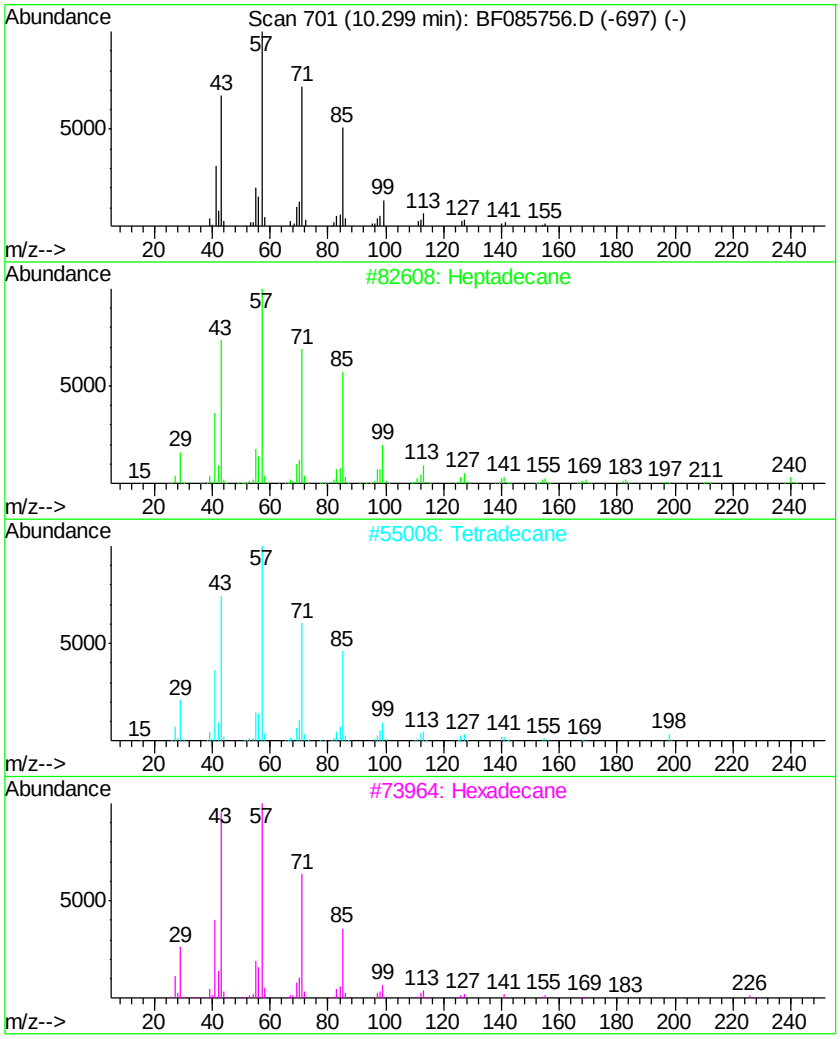
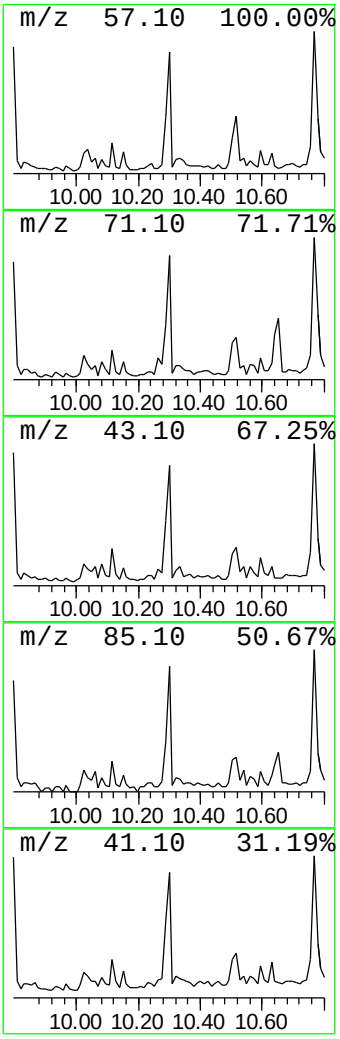
Peak Number 6 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	3.03 ng	116825	Acenaphthene-d10	9.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tetradecane	198	C14H30	000629-59-4	87
3	Hexadecane	226	C16H34	000544-76-3	86
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	80
5	Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	80





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Sample : H1858-03
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-13A

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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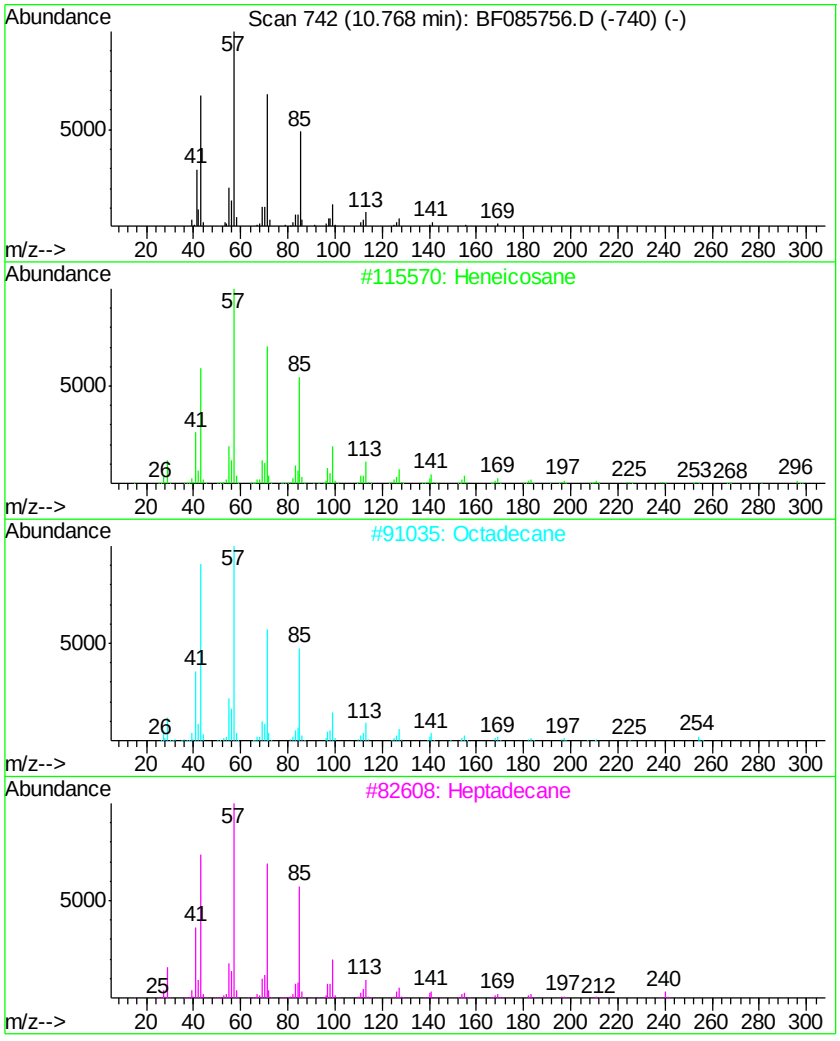
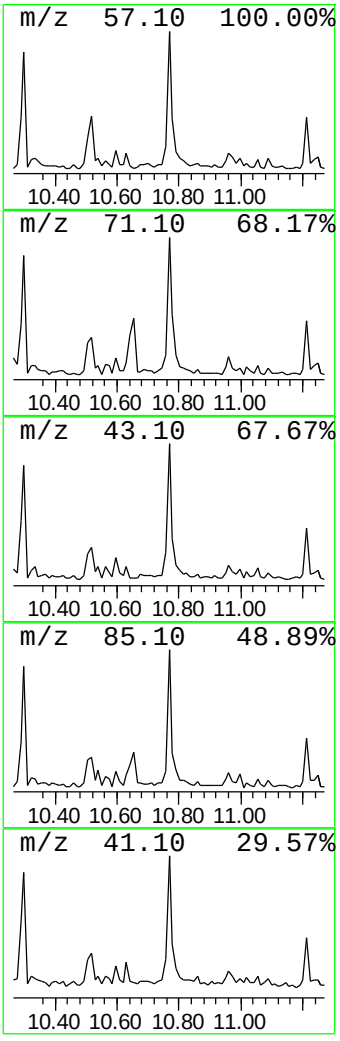
Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	4.17 ng	127547	Phenanthrene-d10	11.34

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





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

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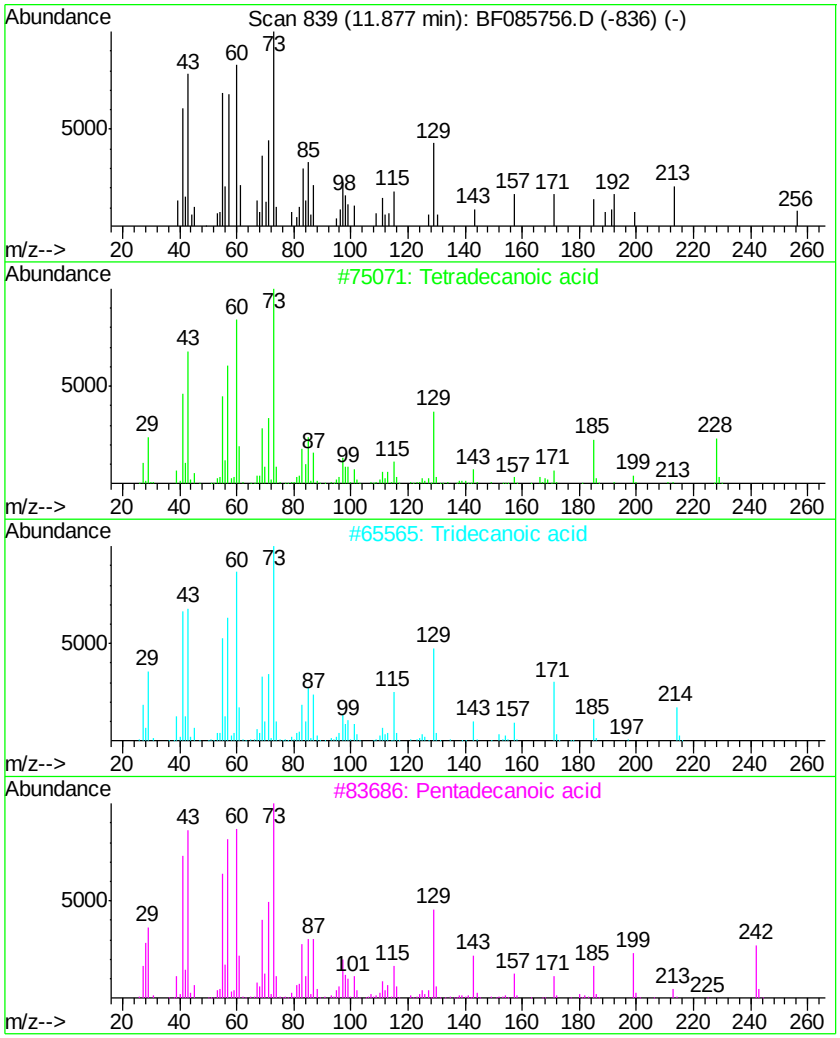
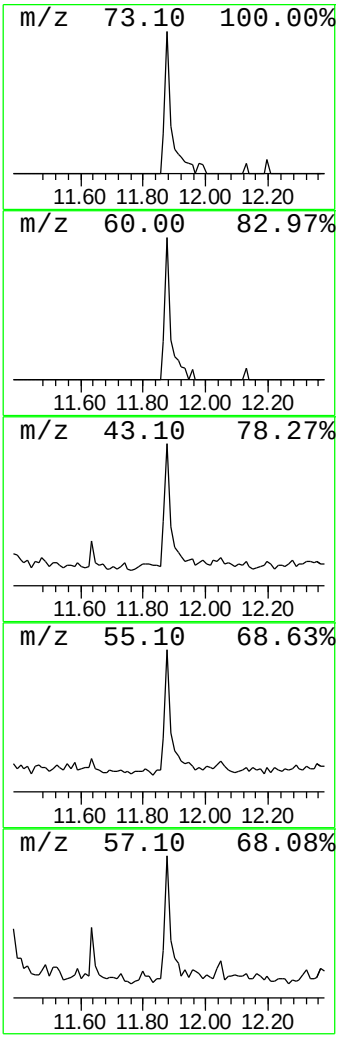
Peak Number 8 Tetradecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.03 ng	62151	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	22





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TIC Library : C:\DATABASE\NIST02.L
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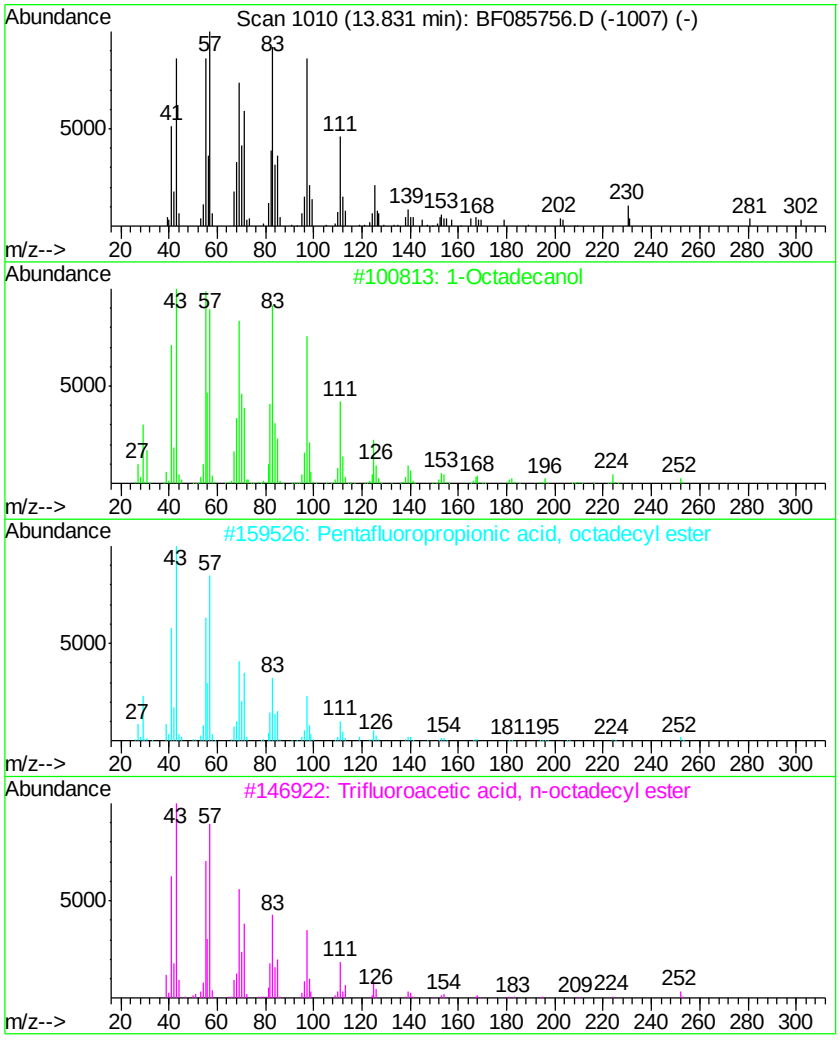
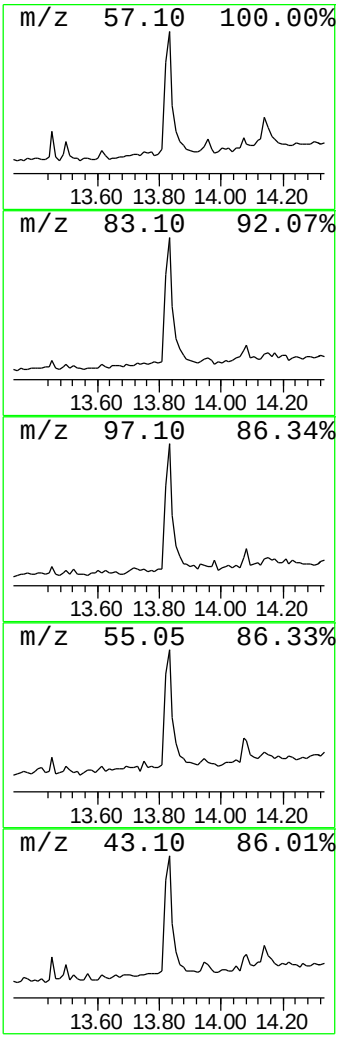
Peak Number 9 1-Octadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	6.04 ng	205422	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	91
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4	Cyclohexadecane	224	C16H32	000295-65-8	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





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TIC Library : C:\DATABASE\NIST02.L
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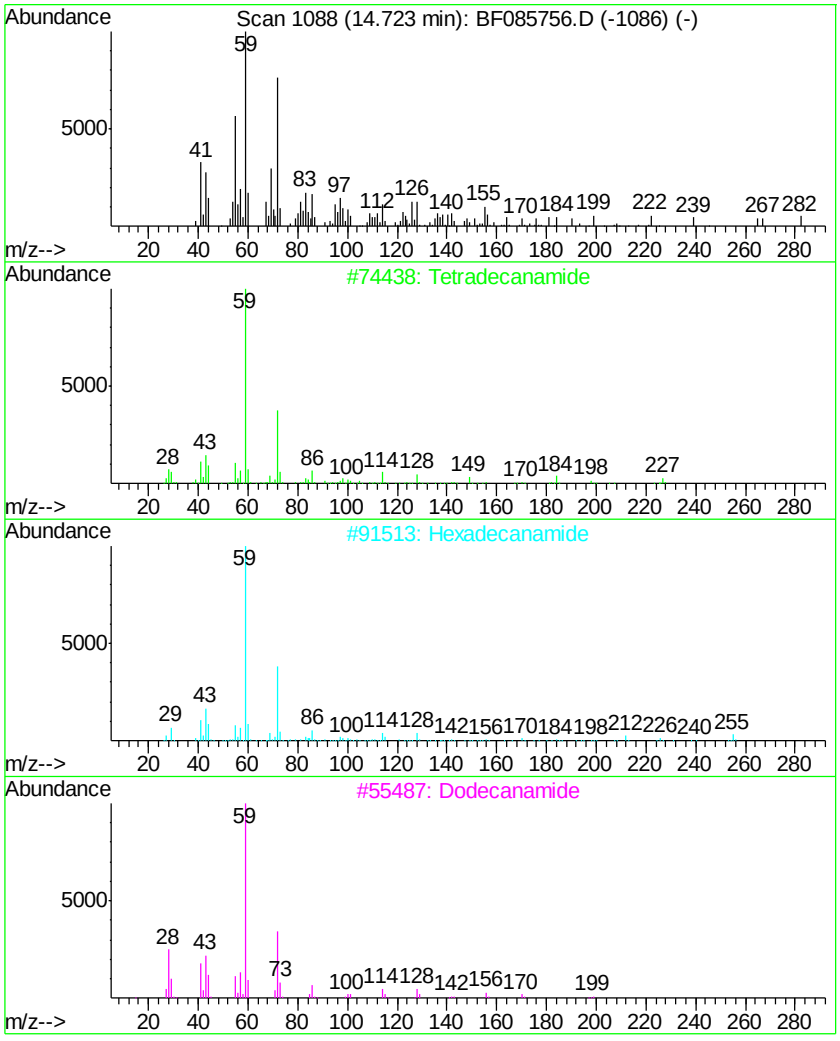
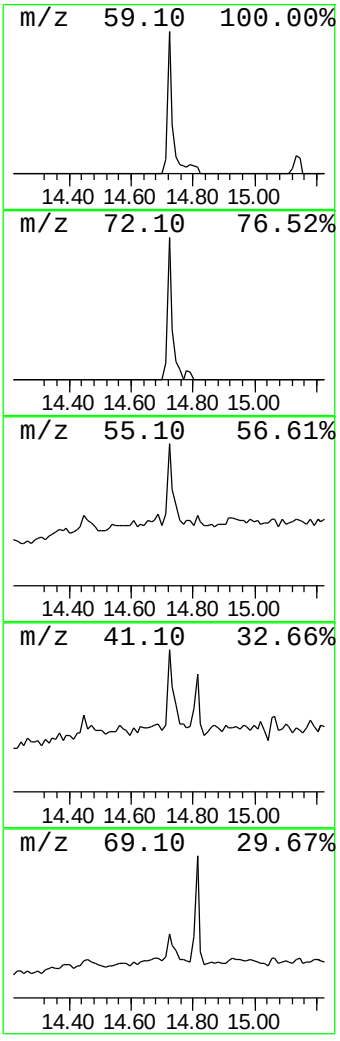
Peak Number 10 Tetradecanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.22 ng	97613	Perylene-d12	15.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	59
2	Hexadecanamide	255	C16H33NO	000629-54-9	50
3	Dodecanamide	199	C12H25NO	001120-16-7	50
4	7-Nonenamide	155	C9H17NO	090949-53-4	49
5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	38





Tentatively Identified Compound (LSC) summary

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Data File : BF085756.D
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Operator : UM/SJ
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Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	30.9	ng	1071200	1	6.82	692768	20.0
2-Pentanone, 4-me...	5.83	3.2	ng	110234	1	6.82	692768	20.0
unknown6.60	6.60	90.2	ng	3125870	1	6.82	692768	20.0
Tetradecane	9.80	2.1	ng	81278	3	9.86	770905	20.0
Heptadecane	10.30	3.0	ng	116825	3	9.86	770905	20.0
Heneicosane	10.77	4.2	ng	127547	4	11.34	612192	20.0
Tetradecanoic acid	11.88	2.0	ng	62151	4	11.34	612192	20.0
1-Octadecanol	13.83	6.0	ng	205422	5	13.98	680117	20.0
Tetradecanamide	14.72	3.2	ng	97613	6	15.40	605878	20.0