LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083116\
Data File : BF089947.D
Acq On : 31 Aug 2016 13:44
Operator : UM/SJ
Sample : H4617-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 415LSB2(4)

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-BF083116.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	12	rVB	52558	122642	1.99%	0.230%
2	1.747	12	14	30	rVB	551681	1076846	17.46%	2.016%
3	4.776	276	279	288	rVB	869146	1427042	23.13%	2.672%
4	5.222	314	318	320	rBV	4311243	5476852	88.78%	10.254%
5	6.285	407	411	413	rBV	4483586	5846137	94.77%	10.945%
6	6.399	418	421	424	rVV	4041692	4947330	80.20%	9.262%
7	6.639	439	442	444	rBV	1290989	1430872	23.20%	2.679%
8	6.787	453	455	458	rBV	3191736	3994198	64.75%	7.478%
9	7.199	488	491	494	rBV	2550745	3308271	53.63%	6.194%
10	7.325	498	502	509	rBV	127429	270144	4.38%	0.506%
11	7.919	552	554	556	rBV	2246154	1883256	30.53%	3.526%
12	9.005	645	649	651	rBV	4628726	6168797	100.00%	11.549%
13	9.279	671	673	675	rBV	94192	77052	1.25%	0.144%
14	9.393	681	683	685	rVB	1424370	1160262	18.81%	2.172%
15	9.668	704	707	709	rBV	1852619	2080362	33.72%	3.895%
16	10.114	745	746	748	rVB	110010	102580	1.66%	0.192%
17	10.331	762	765	769	rBV	41444	84604	1.37%	0.158%
18	10.445	772	775	778	rVV	3039862	3132435	50.78%	5.864%
19	10.548	783	784	786	rBV	98640	133409	2.16%	0.250%
20	10.582	786	787	791	rVB	126405	182782	2.96%	0.342%
21	11.028	822	826	828	rBV	89177	108944	1.77%	0.204%
22	11.131	833	835	838	rVV	2024497	1922240	31.16%	3.599%
23	11.382	856	857	862	rVB	255853	258798	4.20%	0.485%
24	11.691	881	884	892	rBV2	139339	269991	4.38%	0.505%
25	12.468	950	952	955	rBV	82201	102620	1.66%	0.192%
26	12.605	961	964	969	rVB2	67652	124758	2.02%	0.234%
27	12.719	971	974	976	rBV	4412429	4321477	70.05%	8.091%
28	13.634	1050	1054	1061	rBV2	115104	201721	3.27%	0.378%
29	13.748	1061	1064	1066	rBV	1664945	1607534	26.06%	3.010%
30	14.102	1092	1095	1096	rBV	51633	62414	1.01%	0.117%
31	14.605	1137	1139	1141	rBV	62117	69277	1.12%	0.130%
32	15.097	1179	1182	1184	rBV	1289179	1458366	23.64%	2.730%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
415LSB2(4)

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-BF083116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

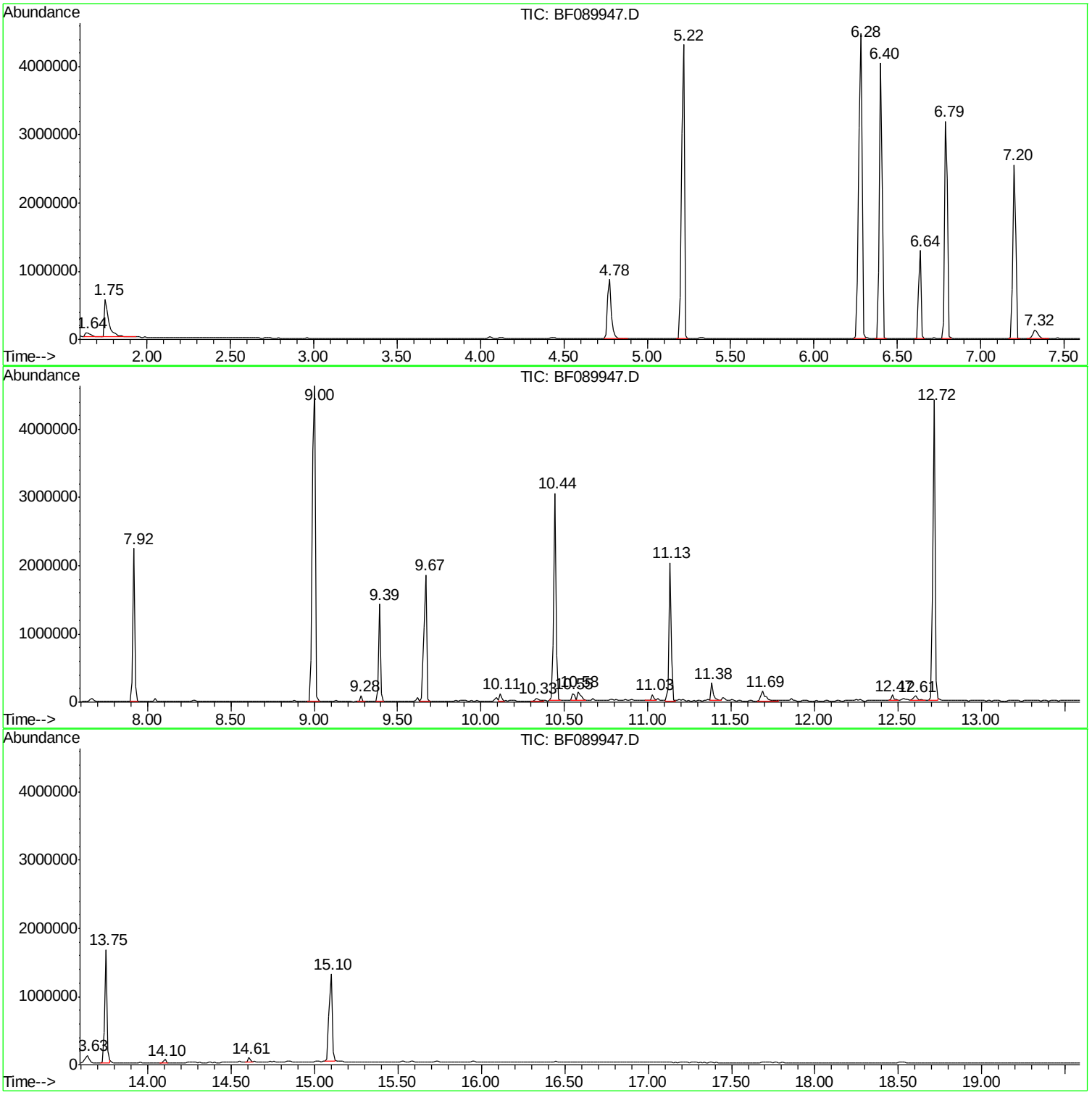
Sum of corrected areas: 53414013

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083116\
Data File : BF089947.D
Acq On : 31 Aug 2016 13:44
Operator : UM/SJ
Sample : H4617-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
415LSB2(4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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Operator : UM/SJ
Sample : H4617-02
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Instrument : BNA_F
ClientSampleId : 415LSB2(4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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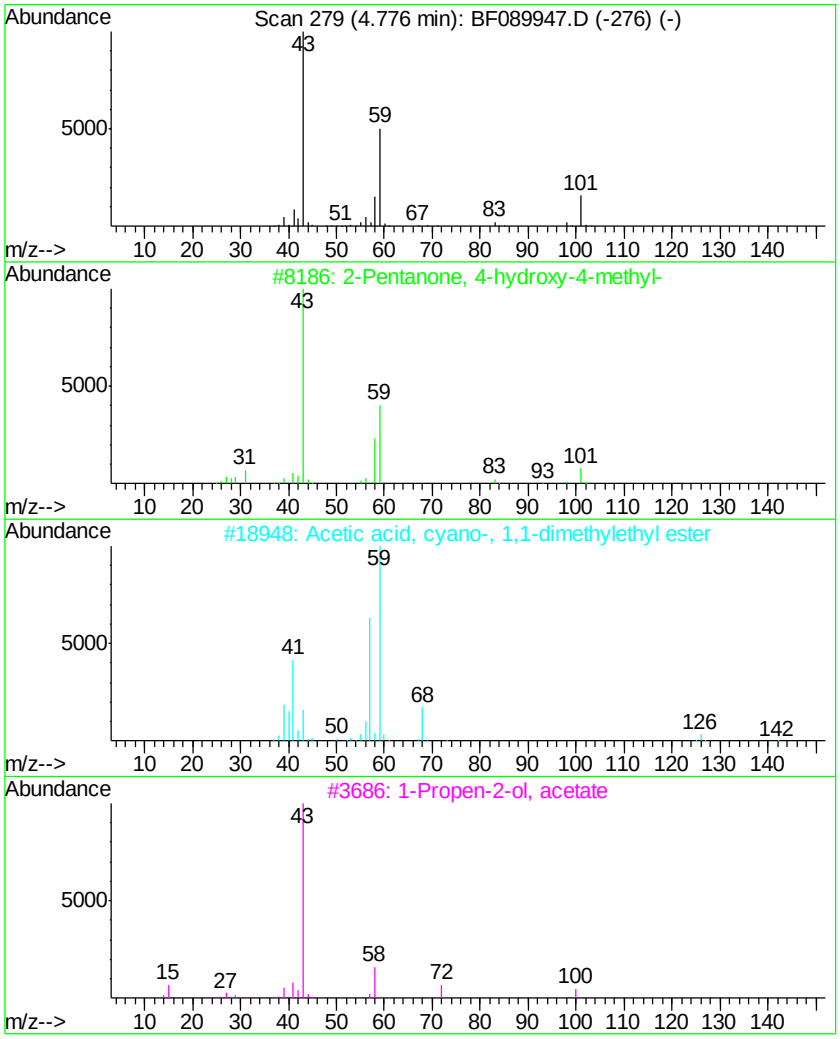
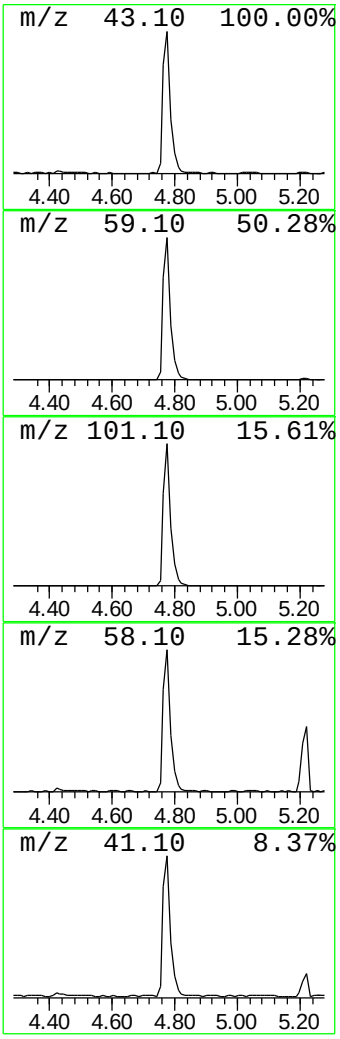
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	19.95 ng	1427040	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF083116\
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Acq On : 31 Aug 2016 13:44
Operator : UM/SJ
Sample : H4617-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 415LSB2(4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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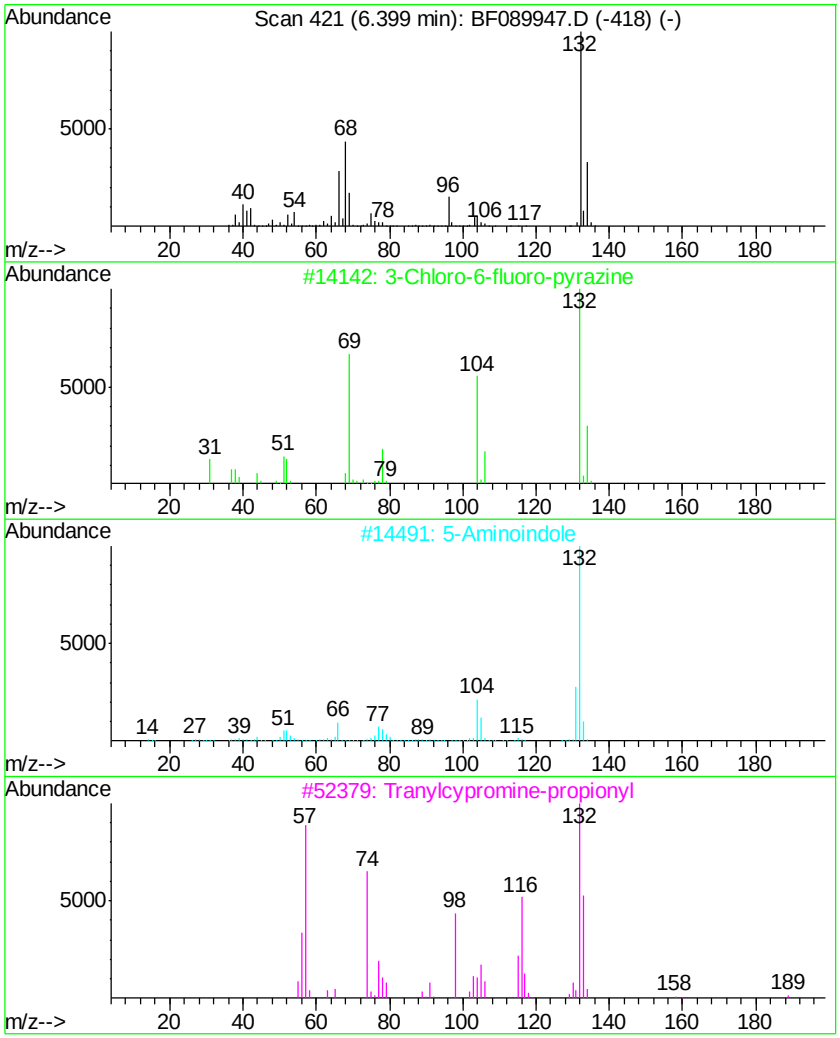
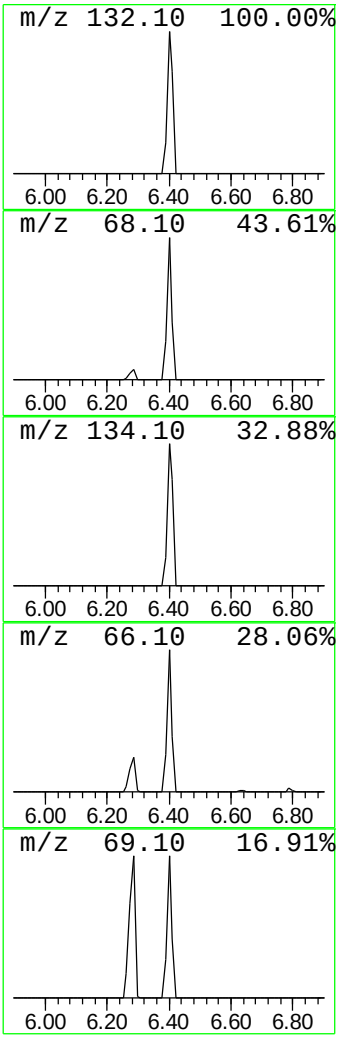
Peak Number 3 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	69.15 ng	4947330	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Operator : UM/SJ
Sample : H4617-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 415LSB2(4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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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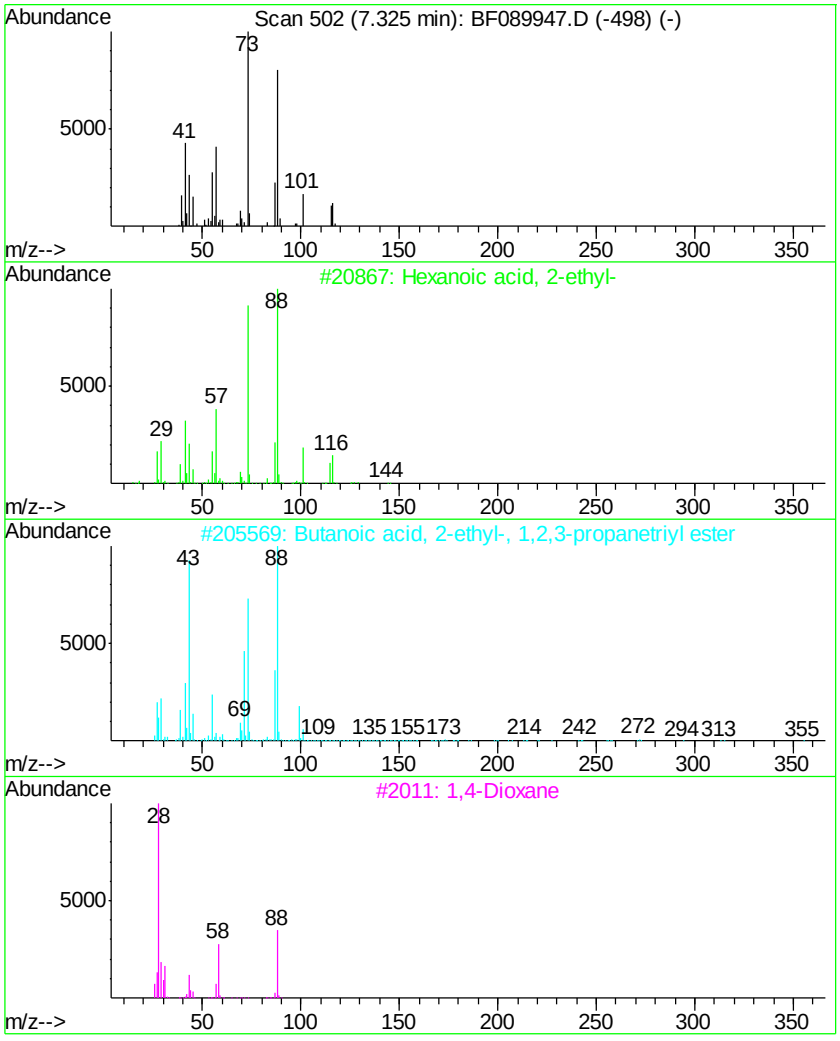
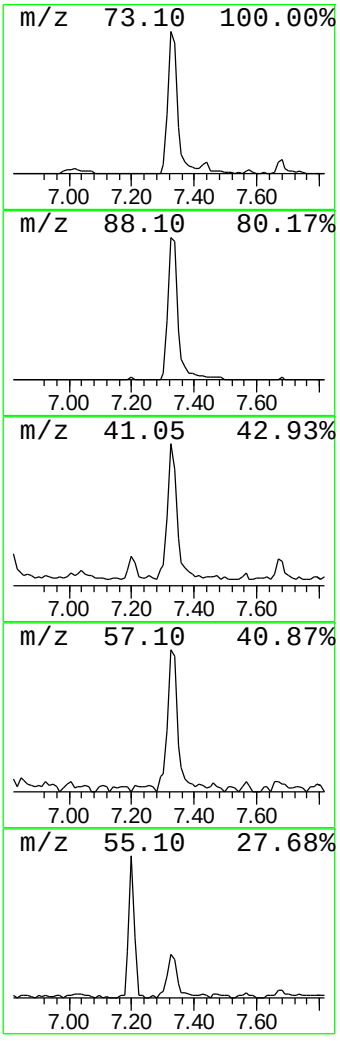
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	2.87 ng	270144	Naphthalene-d8	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3	1,4-Dioxane	88	C4H8O2	000123-91-1	47
4	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
5	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	40





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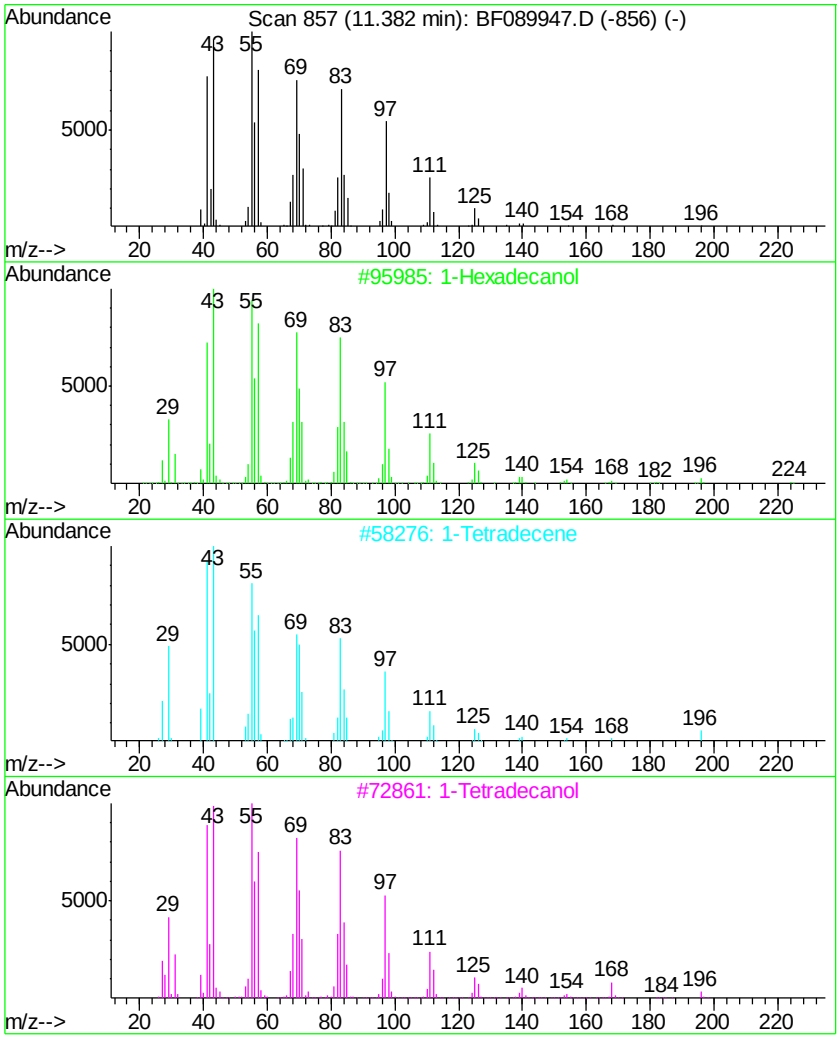
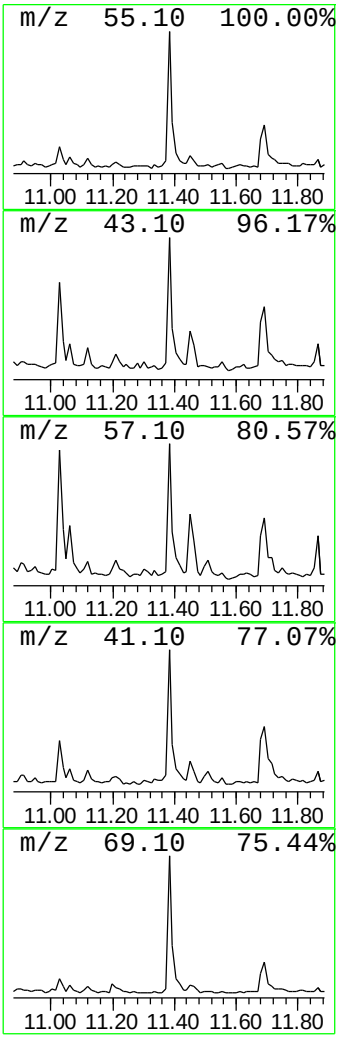
Peak Number 6 1-Hexadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.38	2.69 ng	258798	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	1-Tetradecene	196	C14H28	001120-36-1	91
3	1-Tetradecanol	214	C14H30O	000112-72-1	91
4	n-Pentadecanol	228	C15H32O	000629-76-5	91
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91





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Instrument : BNA_F
ClientSampleId : 415LSB2(4)

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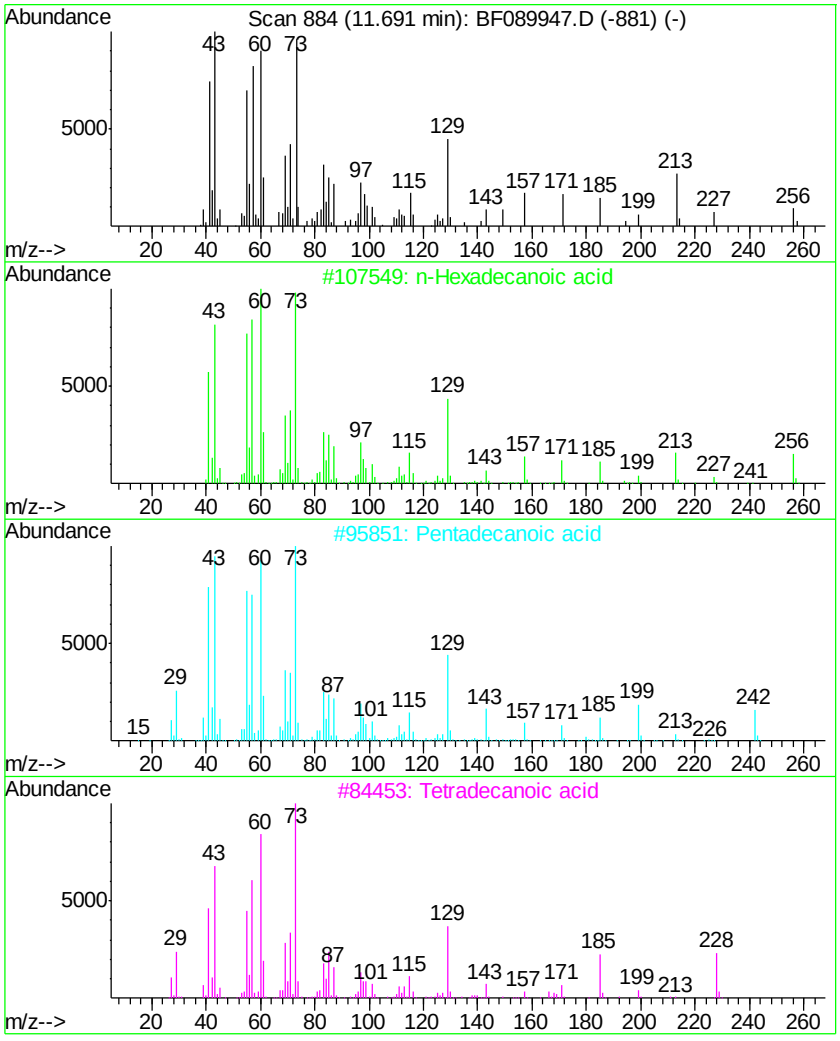
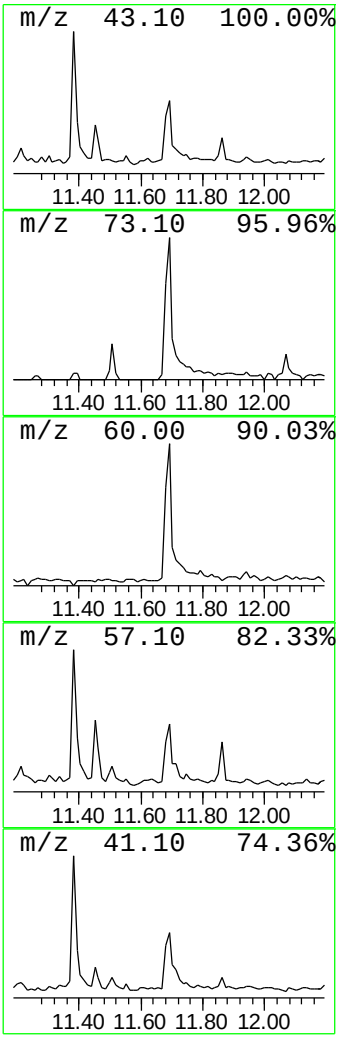
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.81 ng	269991	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	52





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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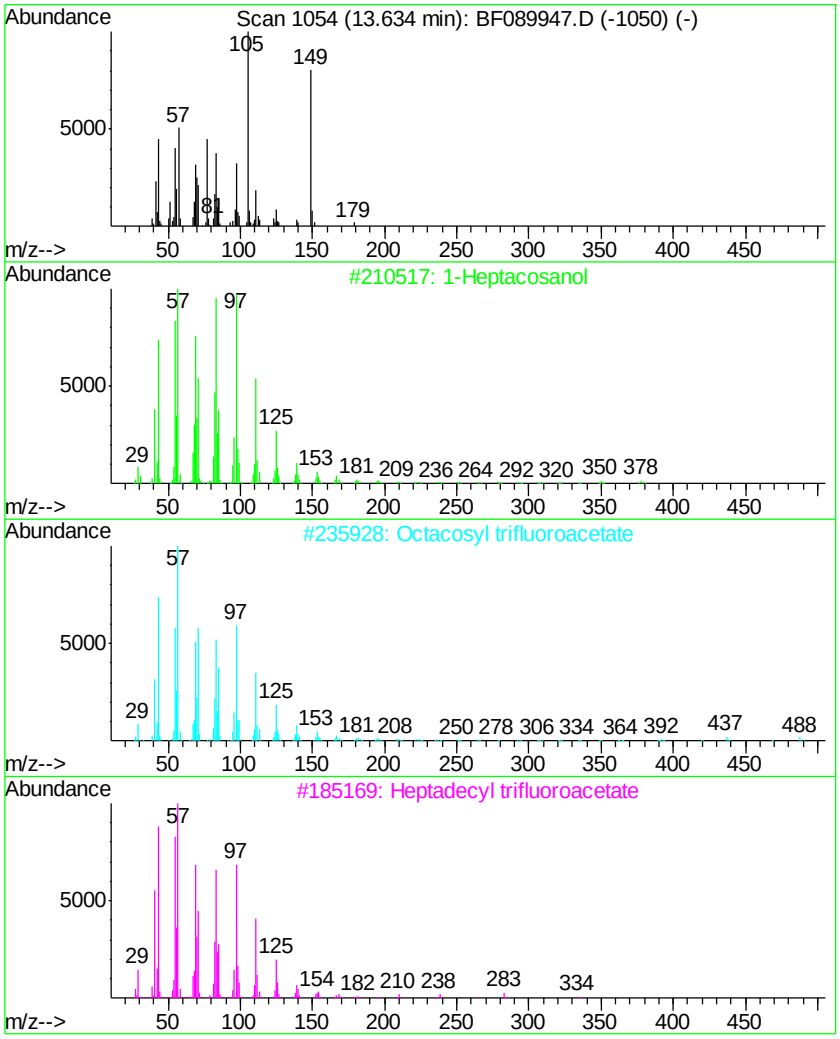
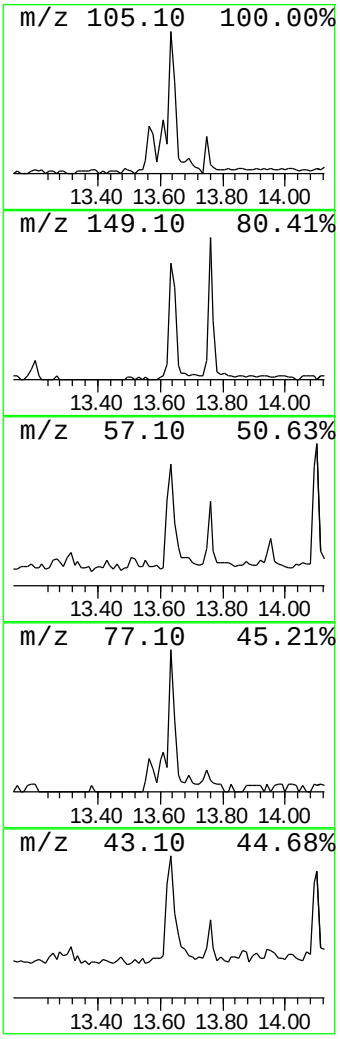
Peak Number 8 unknown13.63 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	2.51 ng	201721	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	42
2	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	42
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	42
4	Octacosanol	410	C28H58O	000557-61-9	42
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	42





Tentatively Identified Compound (LSC) summary

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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...	4.78	19.9	ng	1427040	1	6.64	1430870	20.0
unknown6.40	6.40	69.2	ng	4947330	1	6.64	1430870	20.0
Hexanoic acid, 2-...	7.32	2.9	ng	270144	2	7.92	1883260	20.0
1-Hexadecanol	11.38	2.7	ng	258798	4	11.13	1922240	20.0
n-Hexadecanoic acid	11.69	2.8	ng	269991	4	11.13	1922240	20.0
unknown13.63	13.63	2.5	ng	201721	5	13.75	1607530	20.0