LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030916\
Data File : BF085302.D
Acq On : 9 Mar 2016 16:44
Operator : UM/SJ
Sample : H1623-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

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-BF030316.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	2.390	7	9	11	rVB	4594989	6249895	100.00%	10.180%
2	2.881	50	52	56	rVB	189036	245561	3.93%	0.400%
3	4.447	187	189	192	rVB	227547	258556	4.14%	0.421%
4	5.167	249	252	259	rVB	1049735	1783114	28.53%	2.904%
5	5.567	284	287	290	rBV	3550481	4338322	69.41%	7.066%
6	6.584	372	376	378	rVB	3418443	3994758	63.92%	6.507%
7	6.722	385	388	390	rBV	4087660	4327467	69.24%	7.049%
8	6.950	406	408	410	rBV	1008976	923226	14.77%	1.504%
9	7.110	419	422	424	rBV	3278193	3730386	59.69%	6.076%
10	7.510	454	457	459	rBV	2610394	2802317	44.84%	4.564%
11	7.933	490	494	495	rBV	46780	73076	1.17%	0.119%
12	8.253	517	522	524	rBV2	2013550	2974291	47.59%	4.845%
13	8.299	524	526	528	rVB	133082	125483	2.01%	0.204%
14	8.562	547	549	553	rBV	68184	78198	1.25%	0.127%
15	8.939	580	582	584	rBV	271213	250683	4.01%	0.408%
16	9.042	588	591	593	rBV	136384	120704	1.93%	0.197%
17	9.305	611	614	617	rBV	3932848	5580919	89.30%	9.090%
18	9.990	671	674	675	rBV	1323424	1413819	22.62%	2.303%
19	10.013	675	676	678	rVB	127362	148490	2.38%	0.242%
20	10.185	689	691	694	rVB	129058	133708	2.14%	0.218%
21	10.505	717	719	720	rBV	103840	116925	1.87%	0.190%
22	10.779	740	743	746	rBV	3378137	3619730	57.92%	5.896%
23	11.133	771	774	776	rBV	108968	103233	1.65%	0.168%
24	11.476	801	804	805	rBV	1806998	1745474	27.93%	2.843%
25	11.499	805	806	807	rVB	128021	88268	1.41%	0.144%
26	12.002	846	850	853	rBV	1756290	2178989	34.86%	3.549%
27	12.173	864	865	870	rVB	70250	86840	1.39%	0.141%
28	12.391	882	884	891	rVB	56465	100423	1.61%	0.164%
29	12.711	908	912	915	rBV2	233095	497814	7.97%	0.811%
30	12.802	915	920	922	rVV	3626346	5240301	83.85%	8.535%
31	12.882	925	927	930	rVB2	55406	87343	1.40%	0.142%
32	13.065	940	943	945	rBV	5581579	5920423	94.73%	9.643%
33	13.499	979	981	986	rBV	73488	98859	1.58%	0.161%
34	14.105	1032	1034	1037	rBV2	1025033	1198477	19.18%	1.952%

LSC Area Percent Report

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Data File : BF085302.D
Acq On : 9 Mar 2016 16:44
Operator : UM/SJ
Sample : H1623-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.568	1159	1162	1165	rBV	561571	758194	12.13%	1.235%

Sum of corrected areas: 61394266

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Operator : UM/SJ
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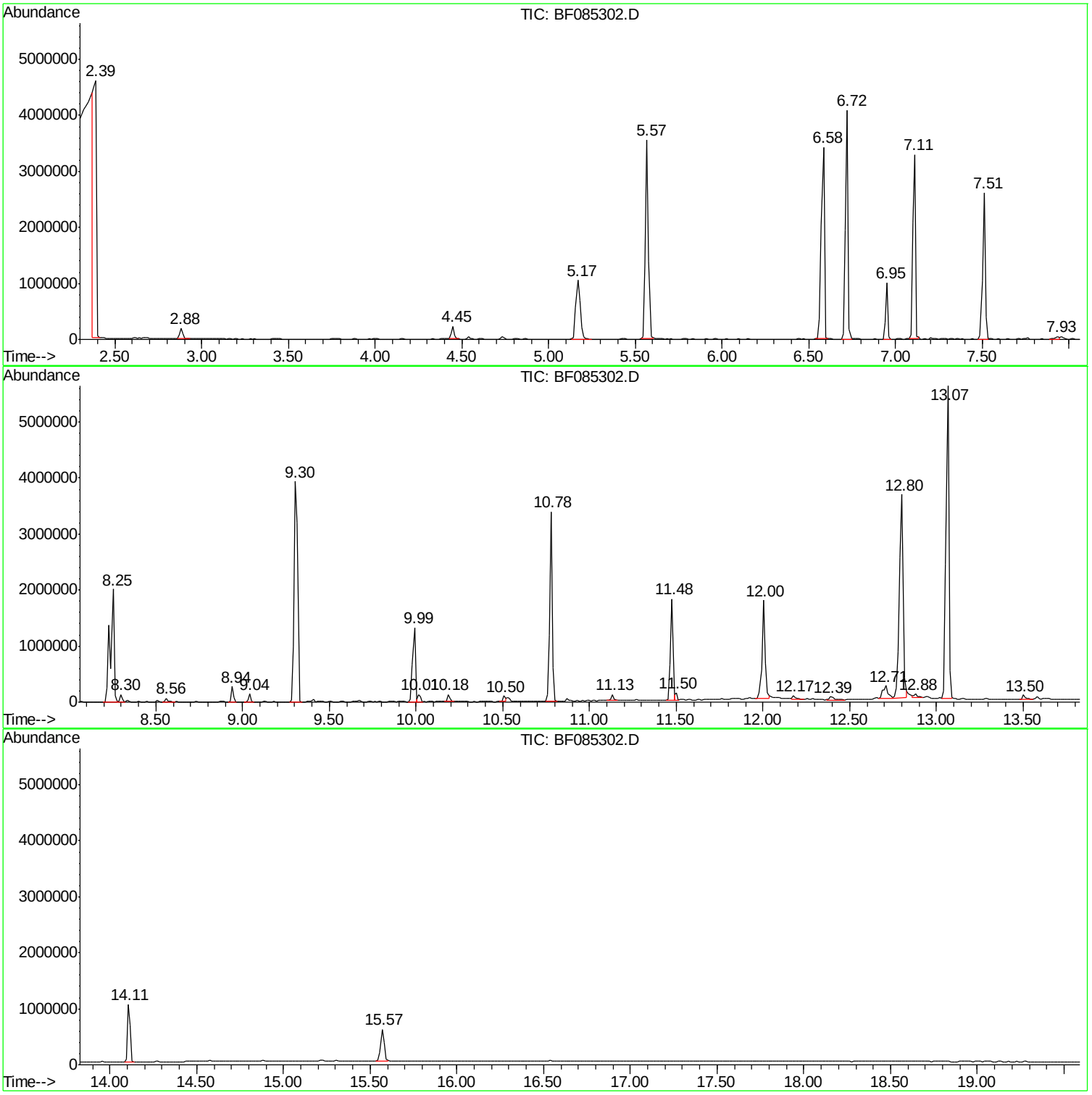
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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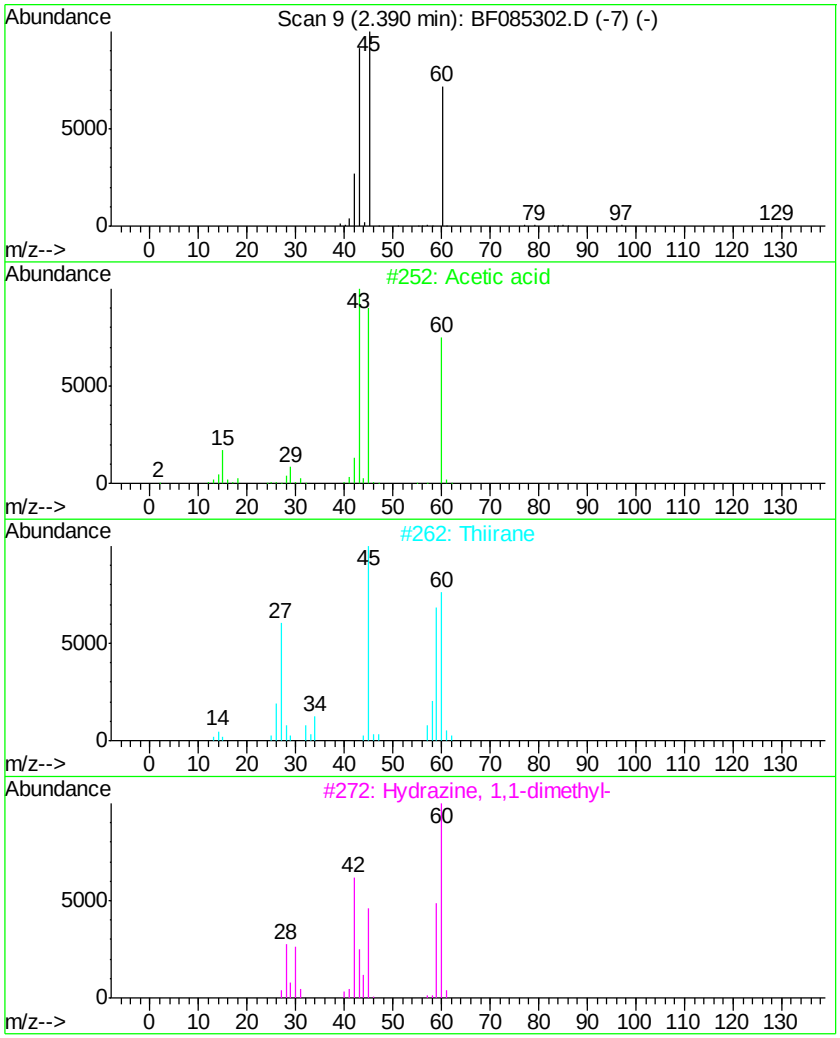
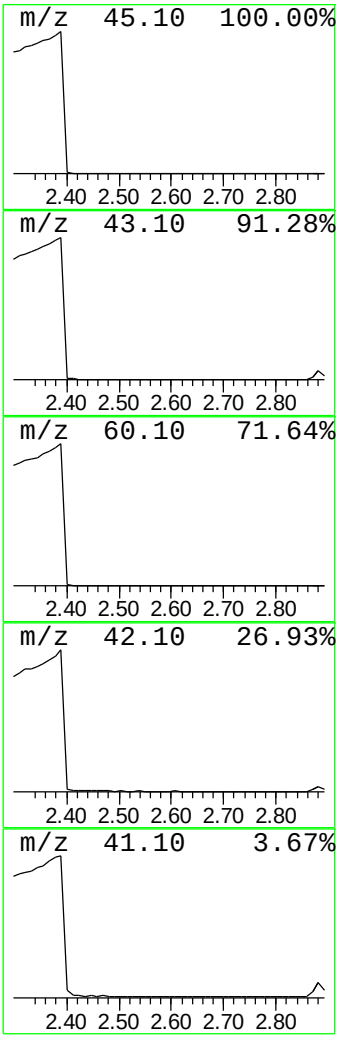
Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.39	135.39 ng	6249900	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	72
2	Thiirane	60	C2H4S	000420-12-2	7
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	4
4	2-Amino-1,3-propanediol	91	C3H9NO2	000534-03-2	4
5	dl-Glyceraldehyde	90	C3H6O3	000056-82-6	4





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Acq On : 9 Mar 2016 16:44
Operator : UM/SJ
Sample : H1623-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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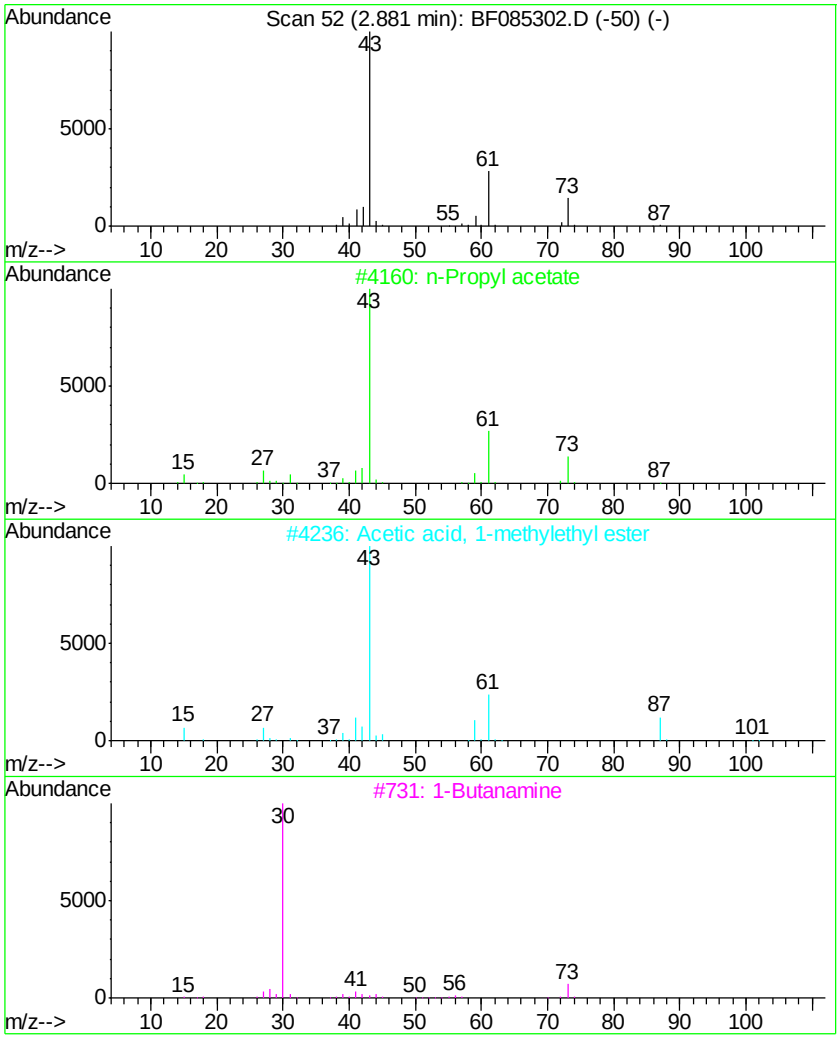
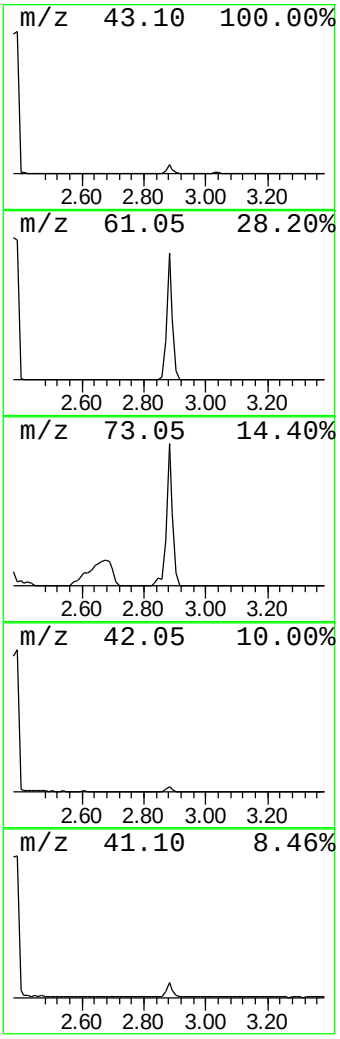
Peak Number 2 n-Propyl acetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	5.32 ng	245561	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	36
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	7
5	Pentane	72	C5H12	000109-66-0	4





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Operator : UM/SJ
Sample : H1623-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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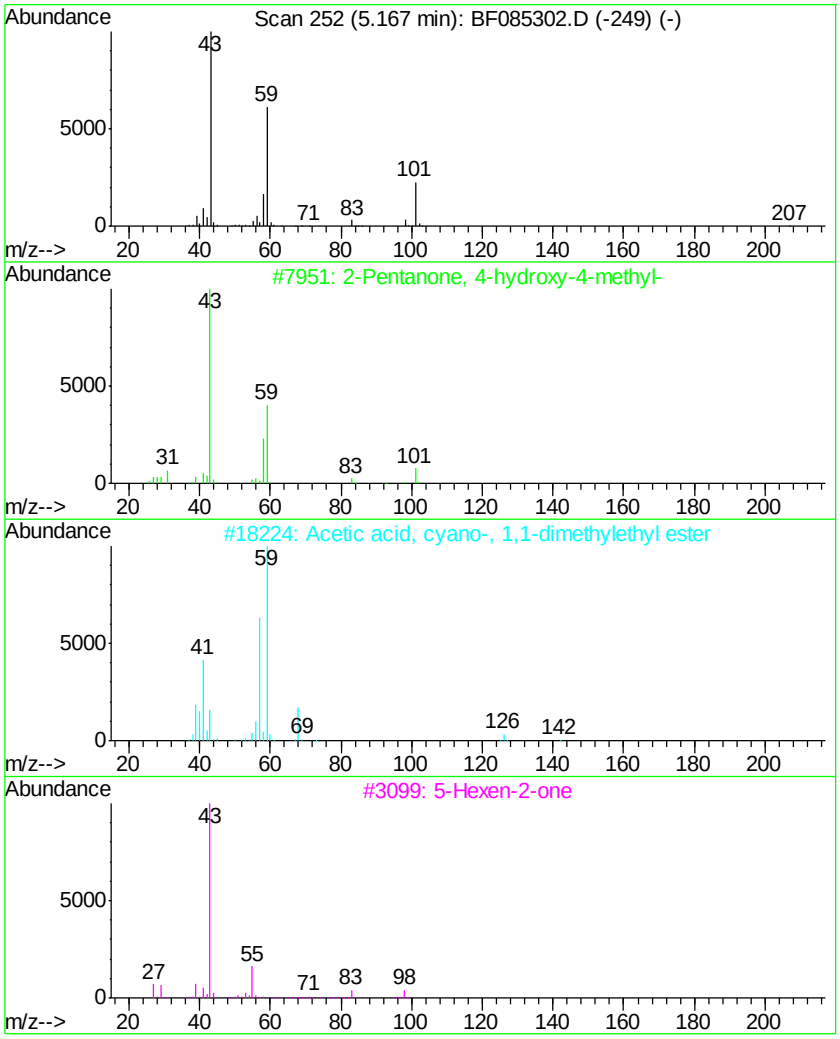
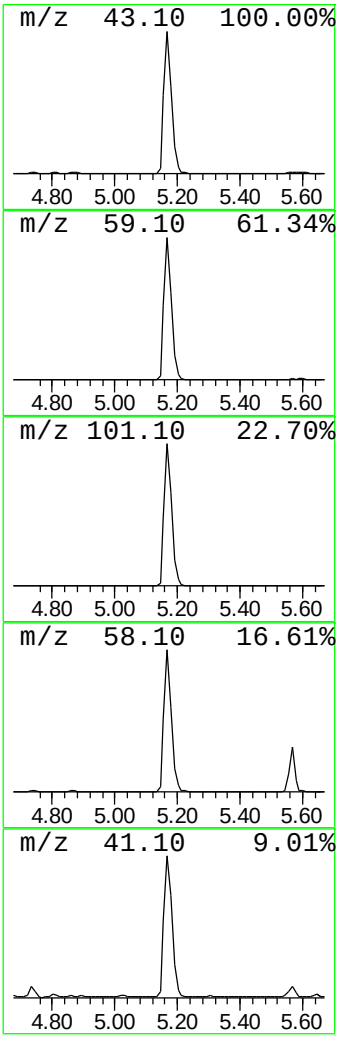
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	38.63 ng	1783110	1,4-Dichlorobenzene-d4	6.95

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	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030916\
Data File : BF085302.D
Acq On : 9 Mar 2016 16:44
Operator : UM/SJ
Sample : H1623-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

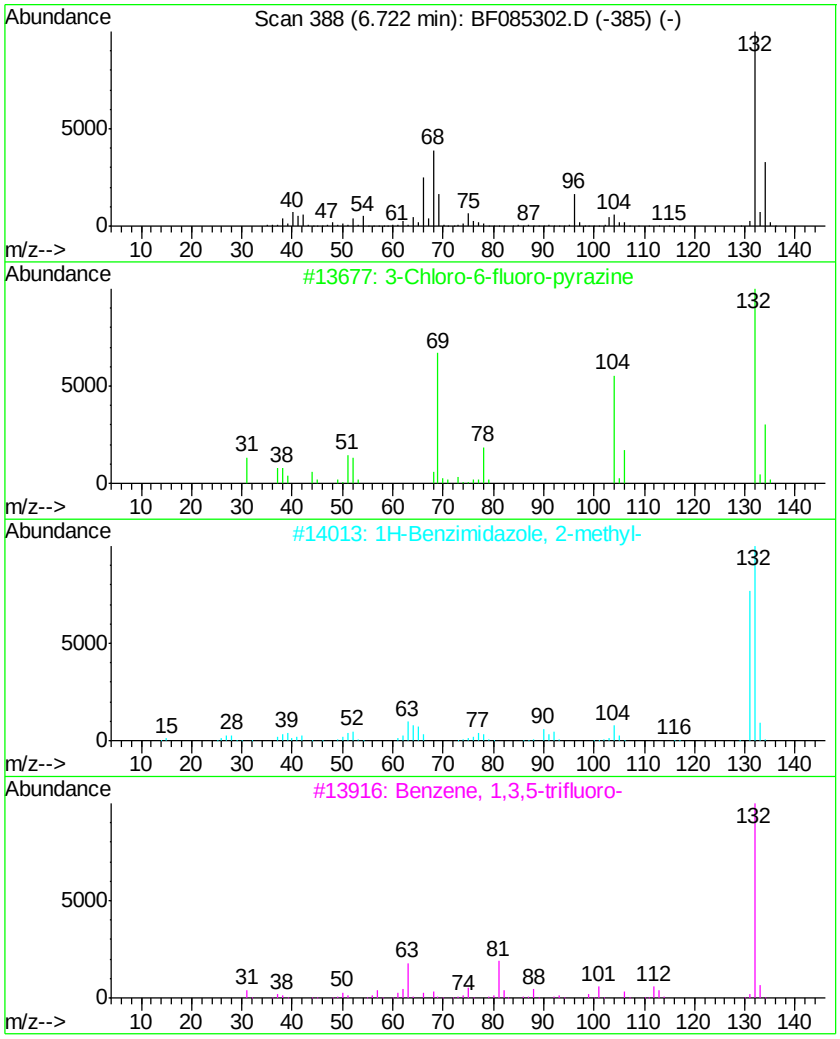
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

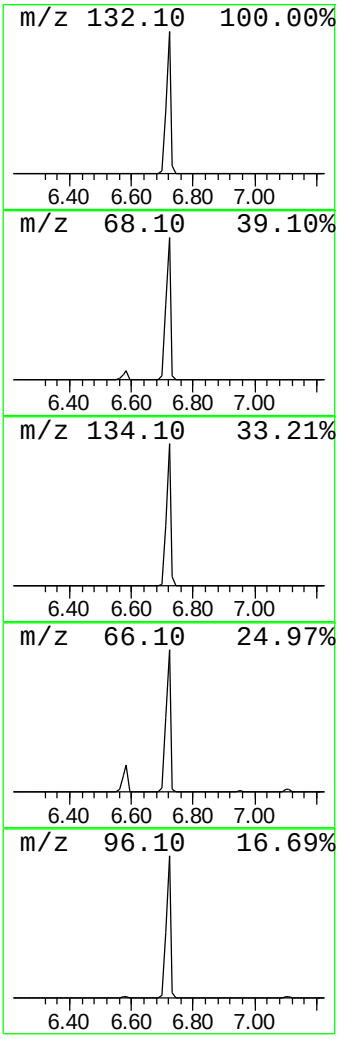
****

Peak Number 5 unknown6.72 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	93.75 ng	4327470	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : H1623-03
Misc :
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Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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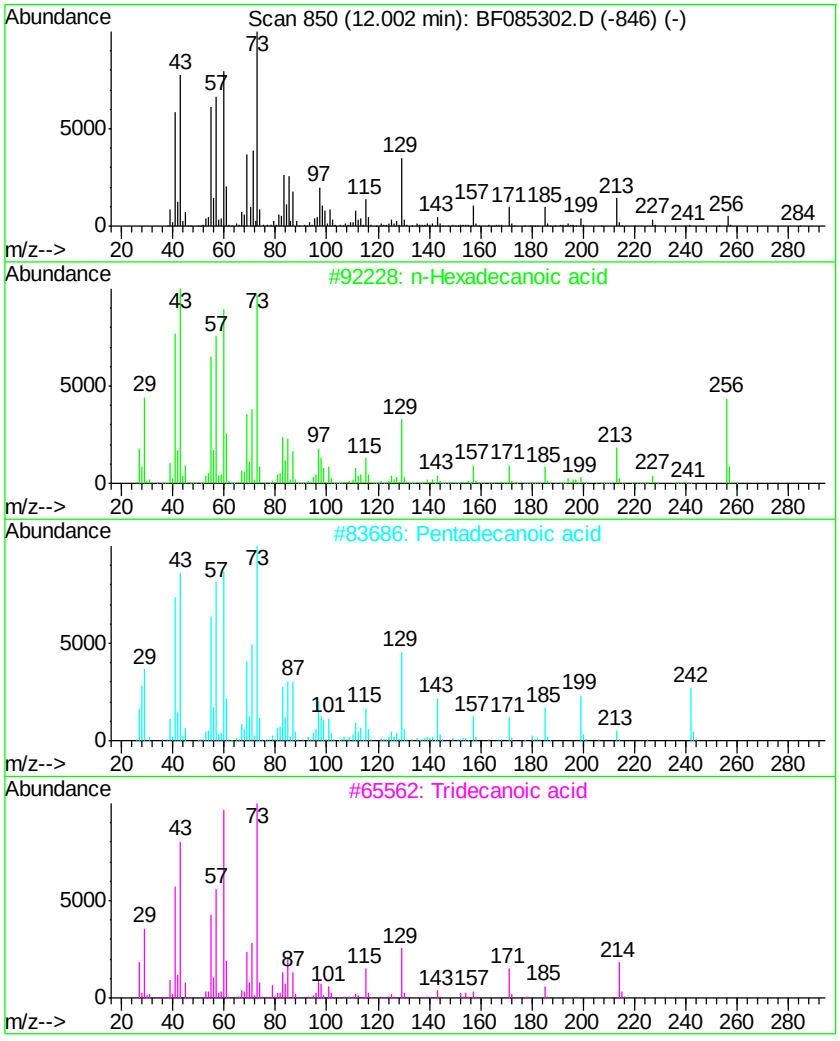
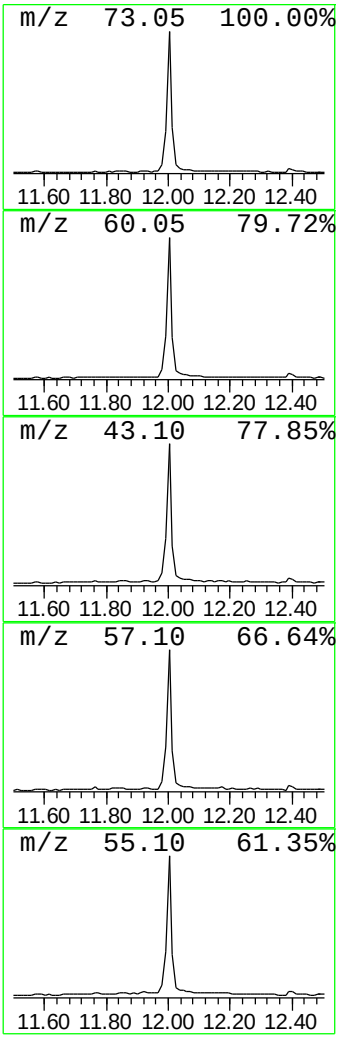
Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	24.97 ng	2178990	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30





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Operator : UM/SJ
Sample : H1623-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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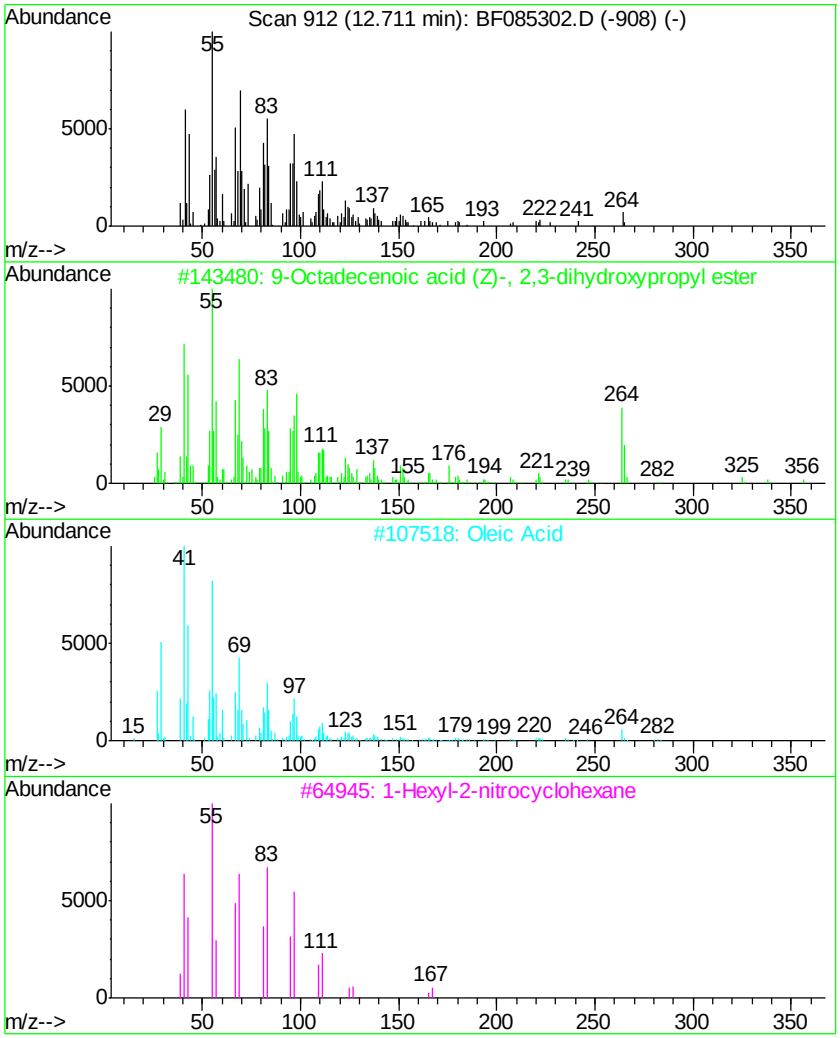
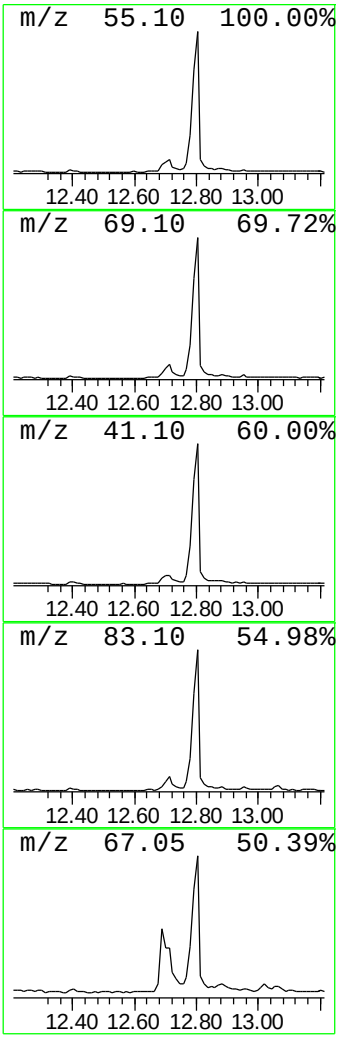
Peak Number 8 9-Octadecenoic acid (Z)-, 2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	5.70 ng	497814	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, 2,3-di...	356	C21H40O4	000111-03-5	81
2	Oleic Acid	282	C18H34O2	000112-80-1	72
3	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	64
4	9-Hexadecenoic acid	254	C16H30O2	002091-29-4	58
5	Trichloroacetic acid, undec-10-e...	314	C13H21Cl3O2	1000280-51-3	53





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Operator : UM/SJ
Sample : H1623-03
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Instrument : BNA_F
ClientSampleId : HSR-WC-30-022516

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

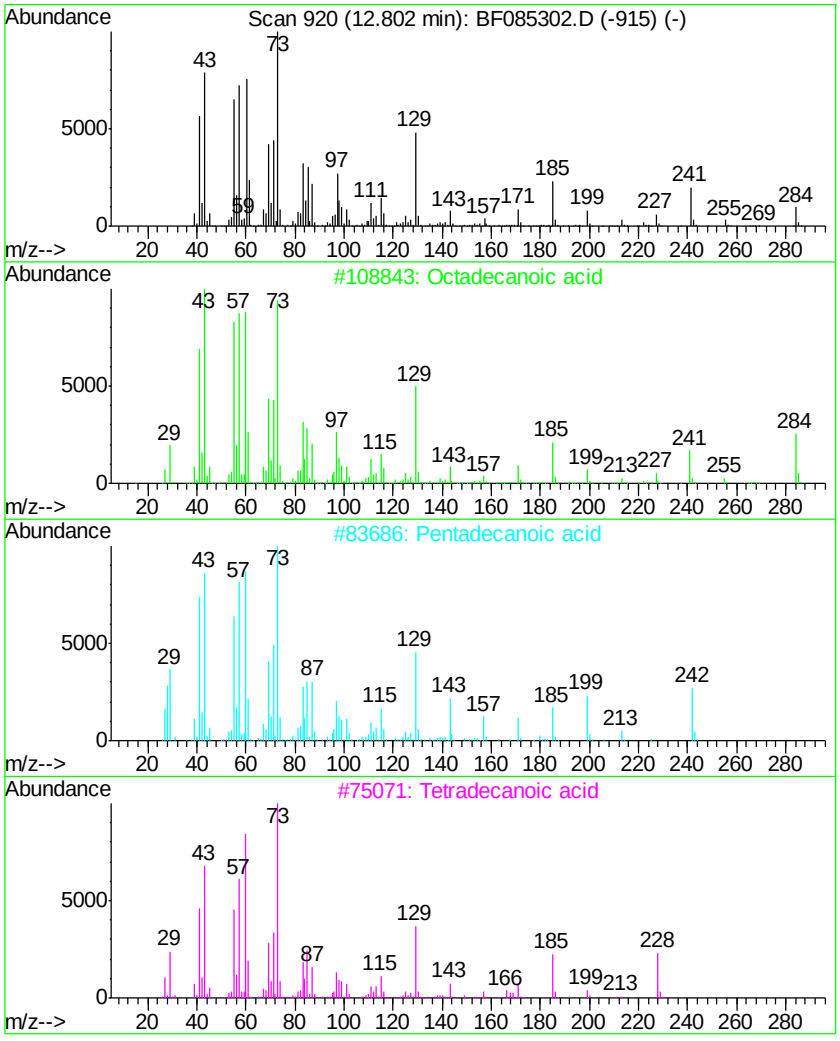
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

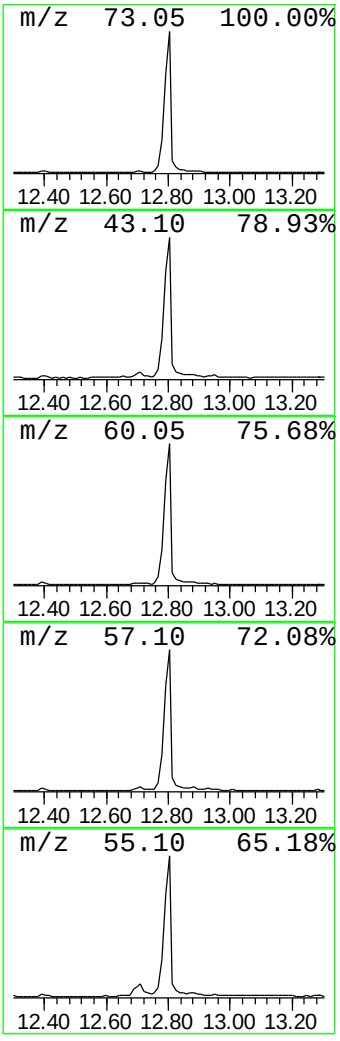
****

Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	87.45 ng	5240300	Chrysene-d12	14.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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
Acetic acid	2.39	135.4	ng	6249900	1	6.95	923226	20.0
n-Propyl acetate	2.88	5.3	ng	245561	1	6.95	923226	20.0
2-Pentanone, 4-hy...	5.17	38.6	ng	1783110	1	6.95	923226	20.0
unknown6.72	6.72	93.8	ng	4327470	1	6.95	923226	20.0
n-Hexadecanoic acid	12.00	25.0	ng	2178990	4	11.48	1745470	20.0
9-Octadecenoic ac...	12.71	5.7	ng	497814	4	11.48	1745470	20.0
Octadecanoic acid	12.80	87.5	ng	5240300	5	14.11	1198480	20.0