LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022947.D
Acq On : 9 Jul 2016 2:05
Operator : UM/SJ
Sample : H3900-01
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1

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_G\METHODS\8270-BG070816.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	3.043	31	35	45	rVB	155727	213986	2.63%	0.415%
2	5.223	402	406	412	rVB	93041	139677	1.72%	0.271%
3	5.699	480	487	497	rBV	1646031	2727866	33.56%	5.289%
4	7.309	754	761	772	rBV	1947515	3381710	41.61%	6.556%
5	7.685	817	825	832	rBV	1750166	3079032	37.88%	5.969%
6	8.155	897	905	911	rBV	409692	684524	8.42%	1.327%
7	8.478	953	960	977	rVB	1278928	2234713	27.49%	4.333%
8	9.324	1095	1104	1113	rBV	1196366	2157237	26.54%	4.182%
9	10.981	1378	1386	1394	rVB	635987	1122430	13.81%	2.176%
10	13.419	1791	1801	1811	rBV	3457094	5447356	67.02%	10.561%
11	14.242	1932	1941	1947	rBV	2938454	4431151	54.52%	8.591%
12	14.800	2029	2036	2045	rVB2	1137577	1885925	23.20%	3.656%
13	16.286	2282	2289	2298	rBV	3398423	5290126	65.09%	10.256%
14	16.480	2318	2322	2331	rVB3	54817	108412	1.33%	0.210%
15	17.555	2497	2505	2511	rBV2	1544448	2352123	28.94%	4.560%
16	18.419	2647	2652	2660	rBV	323718	485555	5.97%	0.941%
17	19.277	2791	2798	2805	rBV9	72164	130943	1.61%	0.254%
18	19.688	2863	2868	2874	rBV3	101566	151130	1.86%	0.293%
19	19.835	2888	2893	2897	rVB	336886	397241	4.89%	0.770%
20	19.947	2909	2912	2917	rVB4	90565	104899	1.29%	0.203%
21	20.158	2941	2948	2953	rBV	5791730	8127764	100.00%	15.758%
22	20.869	3065	3069	3075	rVB2	236698	265012	3.26%	0.514%
23	21.451	3164	3168	3179	rVB	363987	536670	6.60%	1.040%
24	21.844	3229	3235	3247	rVB	1521591	2681132	32.99%	5.198%
25	23.354	3485	3492	3498	rBV4	380787	789726	9.72%	1.531%
26	25.205	3797	3807	3821	rVB2	900761	2653778	32.65%	5.145%

Sum of corrected areas: 51580118

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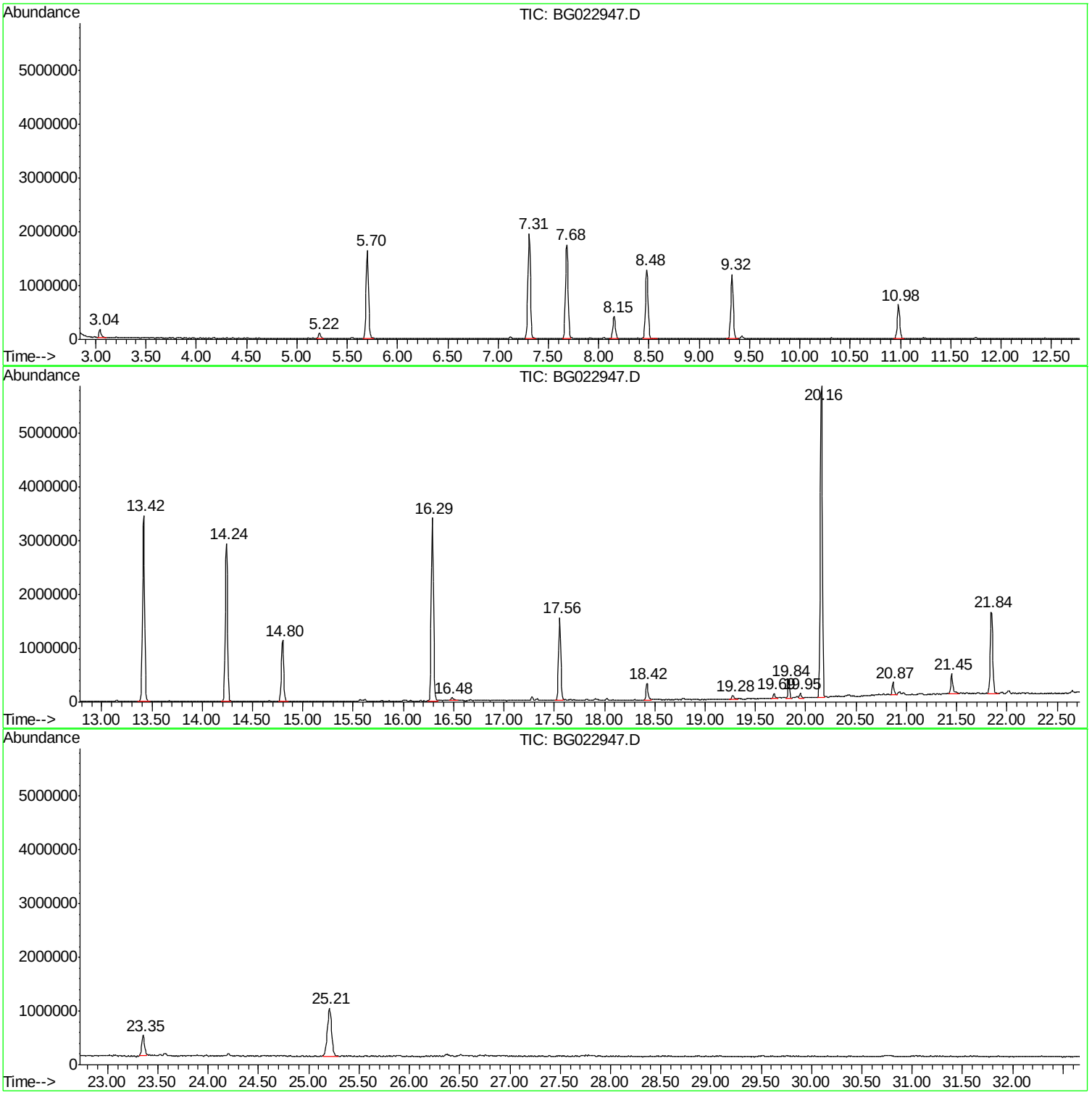
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022947.D
Acq On : 9 Jul 2016 2:05
Operator : UM/SJ
Sample : H3900-01
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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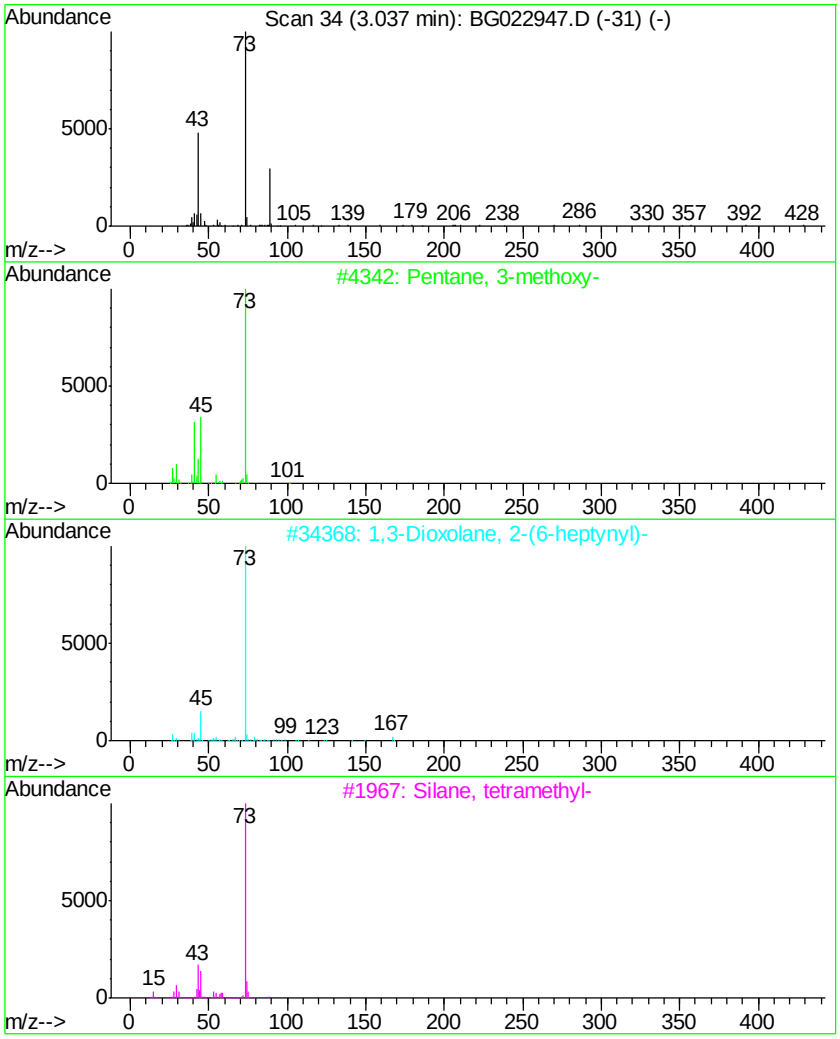
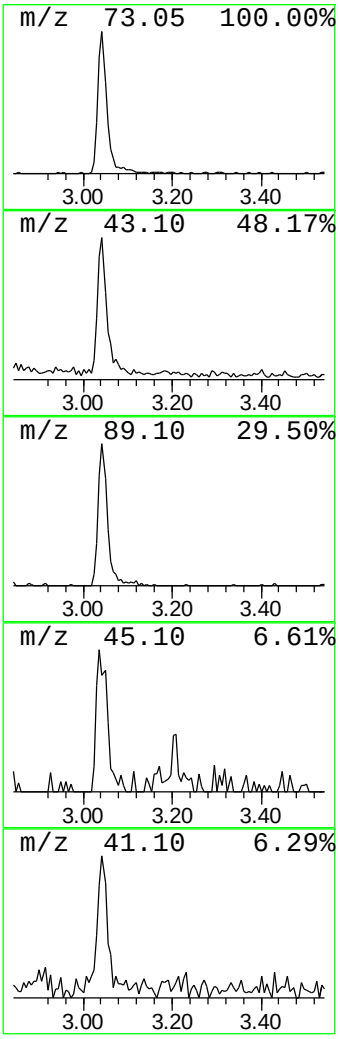
Peak Number 1 unknown3.04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	6.25 ng	213986	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
2	1,3-Dioxolane, 2-(6-heptynyl)-	168	C10H16O2	025595-82-8	9
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4	1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9
5	2,2'-Trimethylenebis-1,3-dioxolane	188	C9H16O4	006543-04-0	9





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Data File : BG022947.D
Acq On : 9 Jul 2016 2:05
Operator : UM/SJ
Sample : H3900-01
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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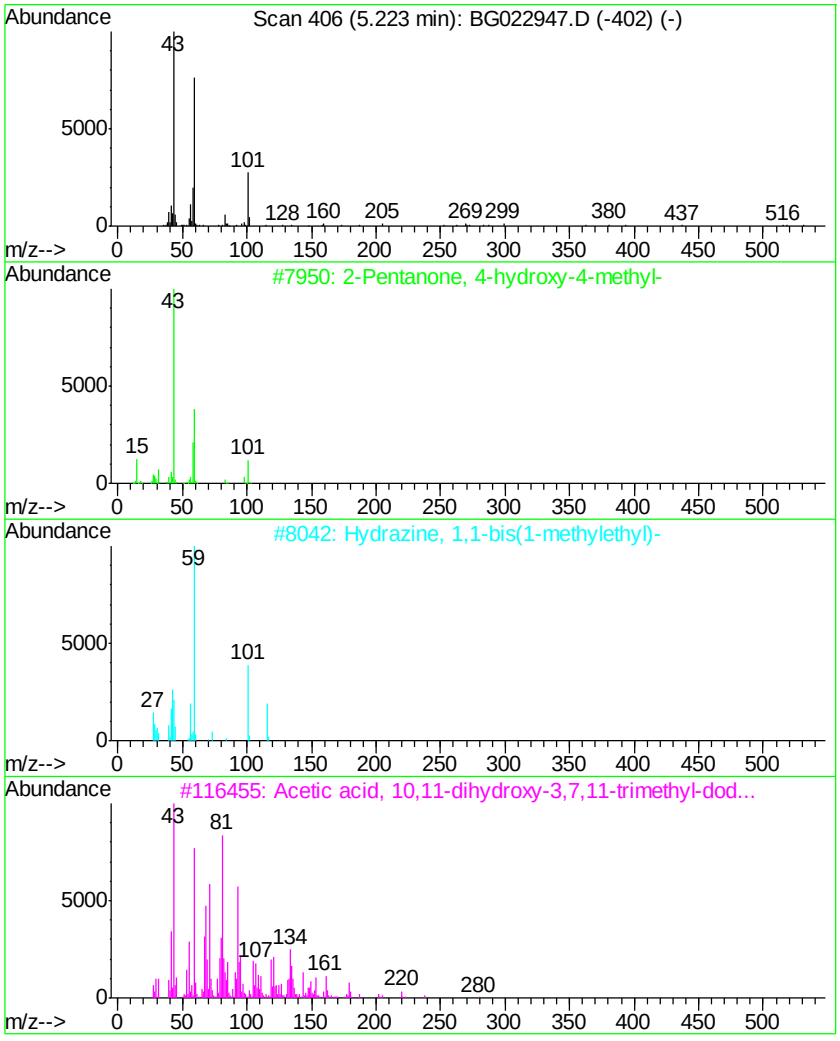
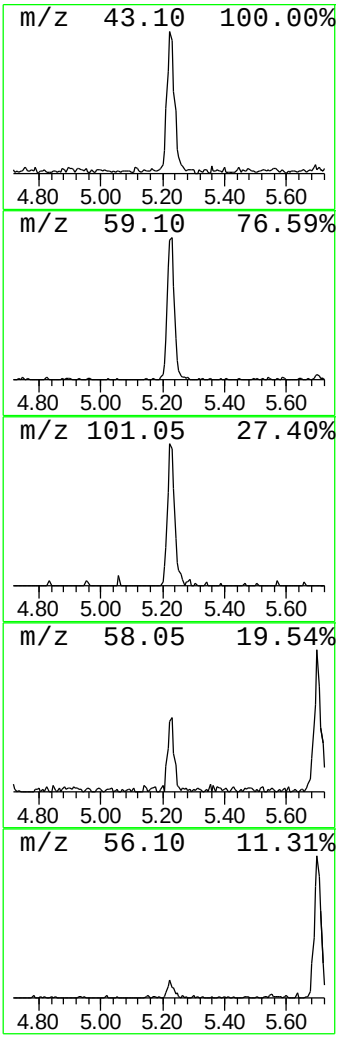
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	4.08 ng	139677	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	37
4	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	36
5	Butanedioic acid, diazo-, dimeth...	172	C6H8N2O4	055514-36-8	36





Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
Data File : BG022947.D
Acq On : 9 Jul 2016 2:05
Operator : UM/SJ
Sample : H3900-01
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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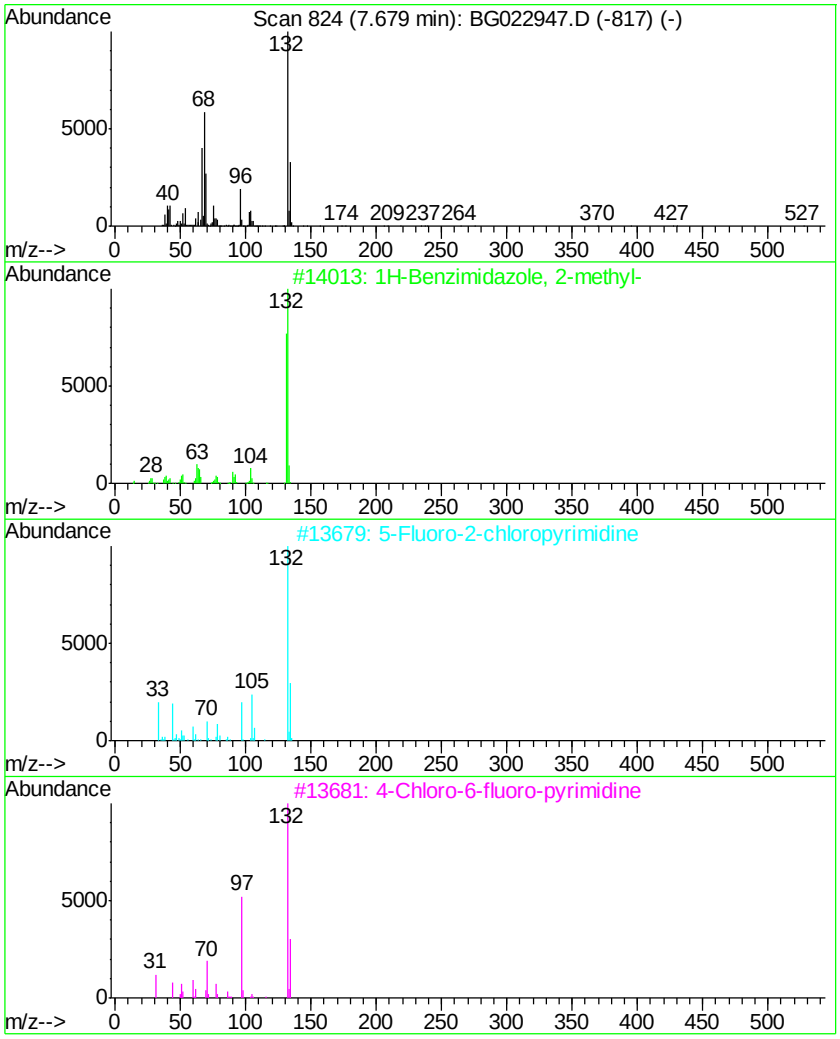
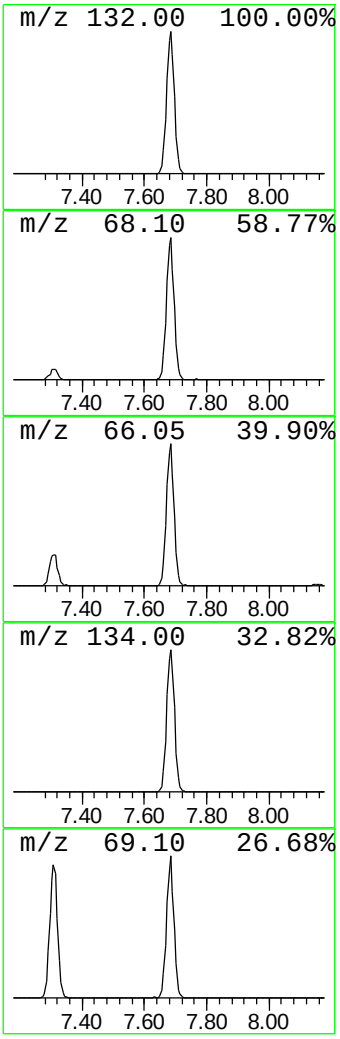
Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	89.96 ng	3079030	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10





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Data File : BG022947.D
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Operator : UM/SJ
Sample : H3900-01
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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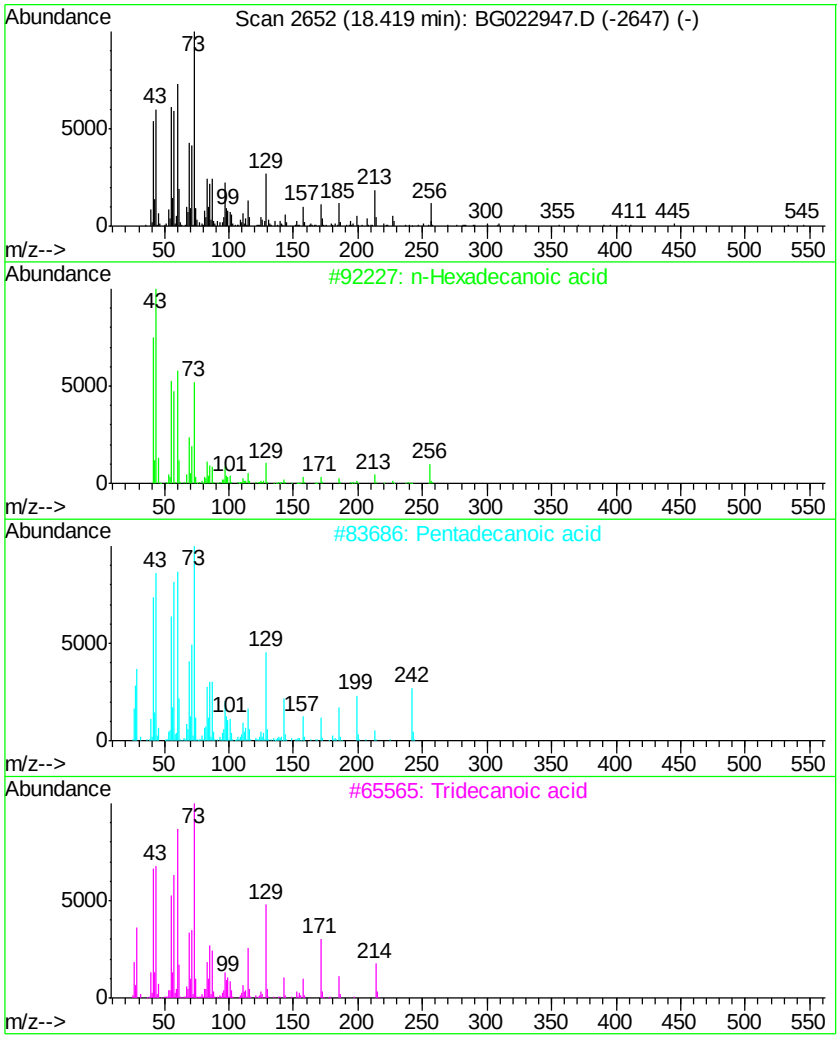
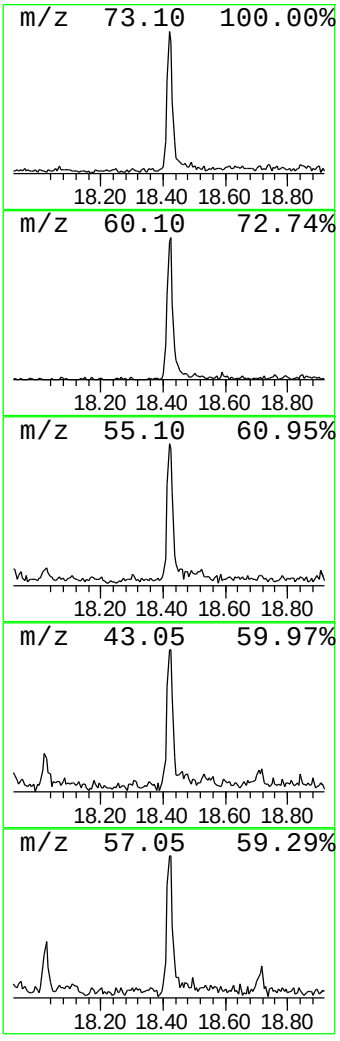
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.13 ng	485555	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	49





Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
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Operator : UM/SJ
Sample : H3900-01
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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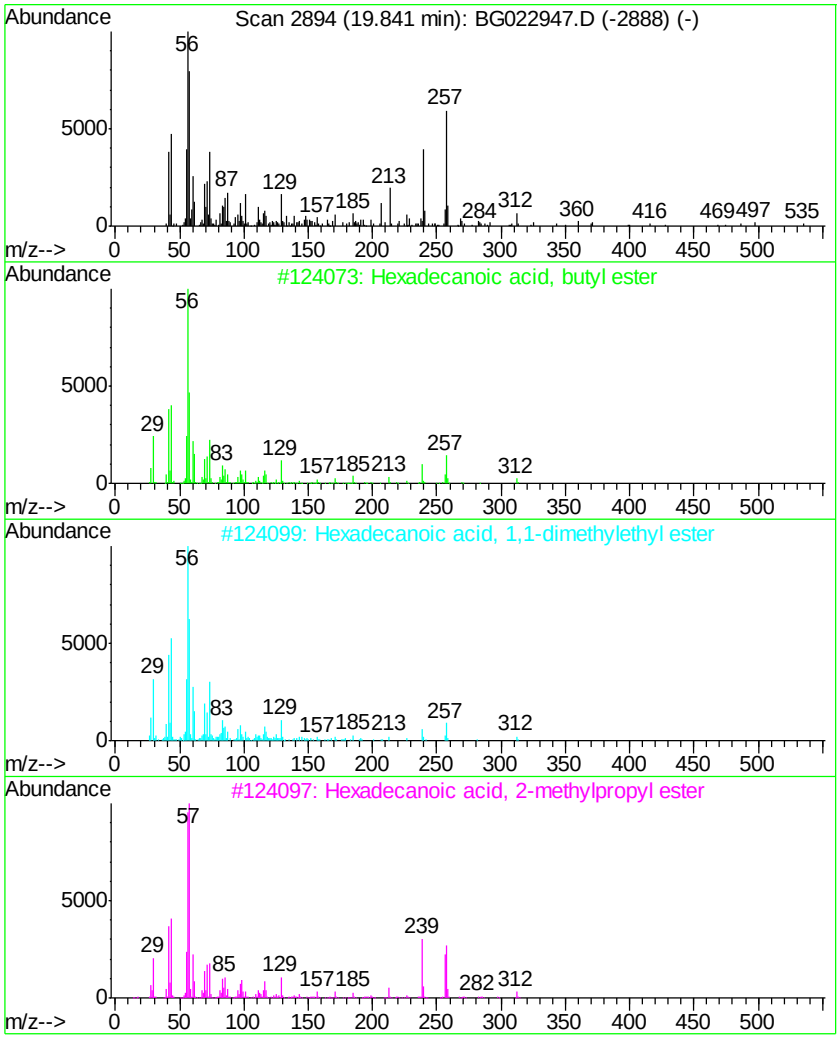
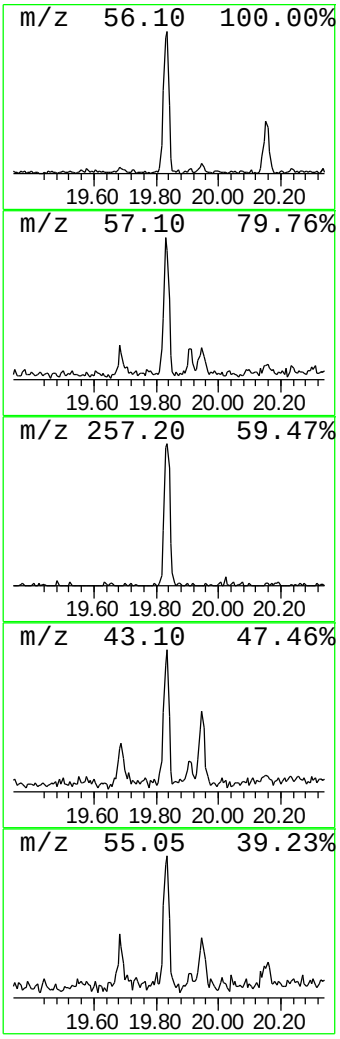
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.84	2.96 ng	397241	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	76
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	46
4	Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38
5	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	32





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Sample : H3900-01
Misc :
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Instrument : BNA_G
ClientSampleId : B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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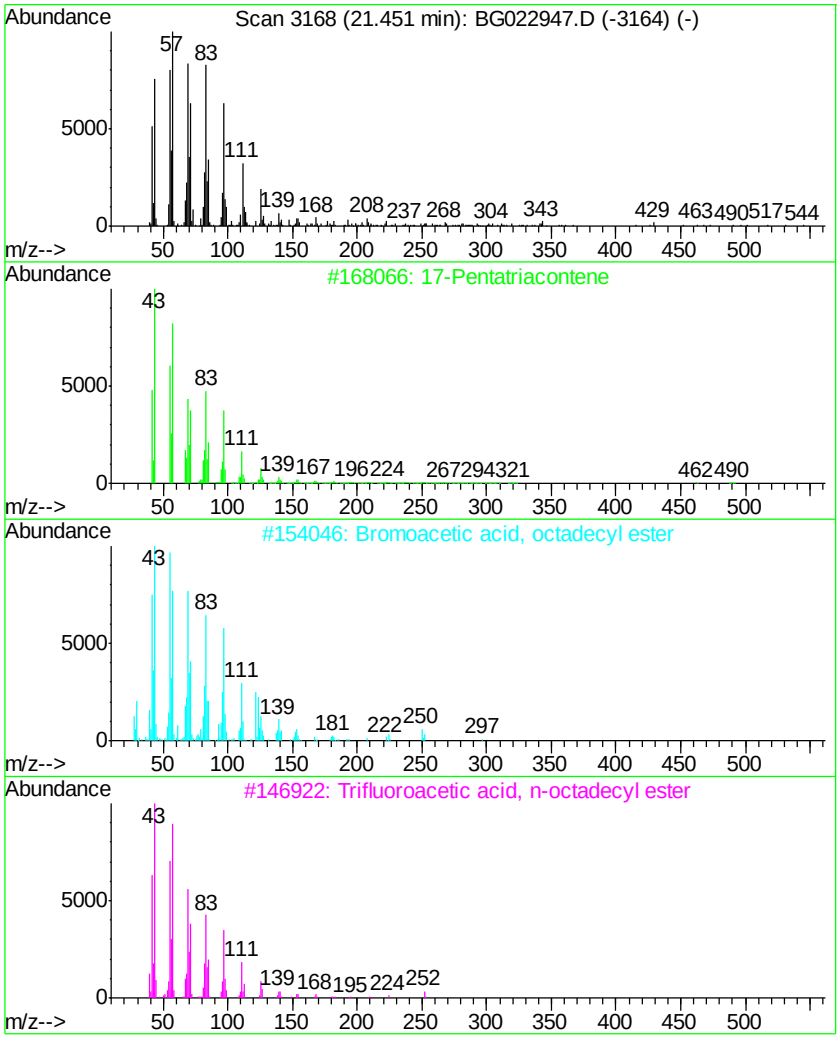
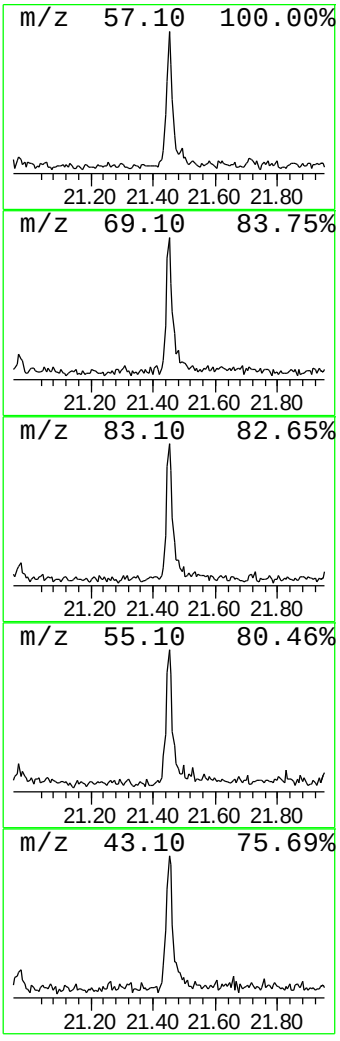
Peak Number 7 17-Pentatriacontene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.45	4.00 ng	536670	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	93
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
5	Cyclotridecane	182	C13H26	000295-02-3	87





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Sample : H3900-01
Misc :
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Instrument : BNA_G
ClientSampleId : B-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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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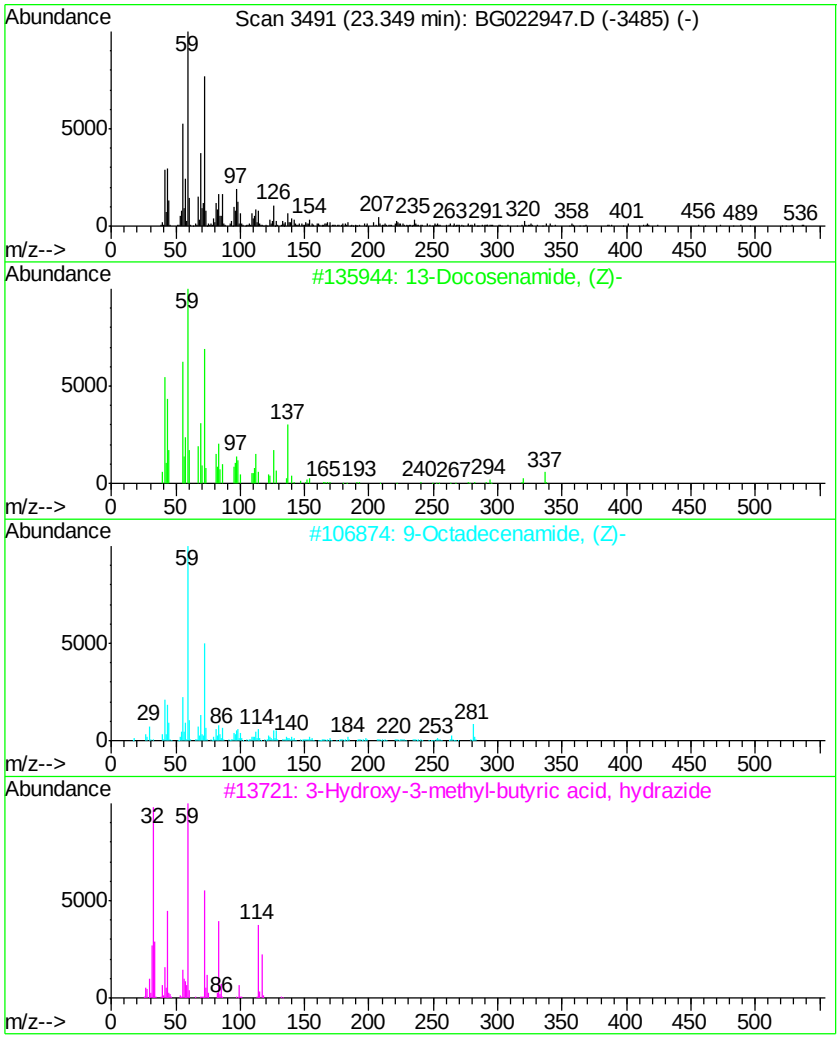
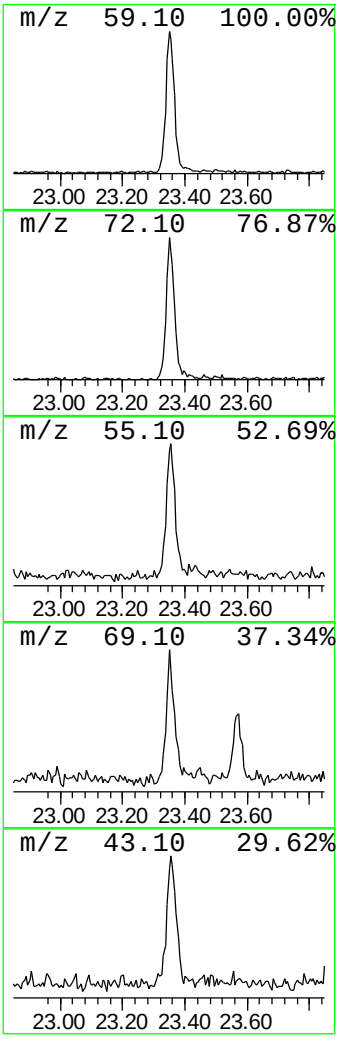
Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	5.89 ng	789726	Chrysene-d12	21.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
3	3-Hydroxy-3-methyl-butyric acid,...	132	C5H12N2O2	1000193-80-2	53
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	47
5	Octadecanamide	283	C18H37NO	000124-26-5	38





Tentatively Identified Compound (LSC) summary

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Operator : UM/SJ
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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
unknown3.04	3.04	6.3	ng	213986	1	8.15	684524	20.0
2-Pentanone, 4-hy...	5.22	4.1	ng	139677	1	8.15	684524	20.0
unknown7.68	7.68	90.0	ng	3079030	1	8.15	684524	20.0
n-Hexadecanoic acid	18.42	4.1	ng	485555	4	17.56	2352120	20.0
Hexadecanoic acid...	19.84	3.0	ng	397241	5	21.84	2681130	20.0
17-Pentatriacontene	21.45	4.0	ng	536670	5	21.84	2681130	20.0
13-Docosenamide, ...	23.35	5.9	ng	789726	5	21.84	2681130	20.0