LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088033.D
Acq On : 15 Jun 2016 8:12
Operator : UM/SJ
Sample : H3473-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1172-(0-4)

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-BF060716.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	1.724	10	12	13	rBV	268243	372185	11.81%	1.561%
2	1.850	21	23	26	rBV	523399	1123852	35.66%	4.714%
3	2.558	82	85	89	rVB	37056	48845	1.55%	0.205%
4	4.970	293	296	311	rVB	185885	328197	10.41%	1.376%
5	5.393	330	333	335	rBV	1955194	2467888	78.31%	10.350%
6	6.422	420	423	426	rBV	1653588	2103657	66.75%	8.823%
7	6.559	432	435	437	rBV	1833051	2561639	81.28%	10.744%
8	6.787	452	455	457	rBV	423460	576439	18.29%	2.418%
9	6.936	466	468	471	rVB	1816530	1917827	60.86%	8.044%
10	7.347	501	504	507	rBV	1438813	1493666	47.40%	6.265%
11	8.067	564	567	569	rBV	958981	814298	25.84%	3.415%
12	9.153	659	662	664	rBV	2673776	3151441	100.00%	13.217%
13	9.816	718	720	723	rBV	622706	784144	24.88%	3.289%
14	10.605	787	789	792	rBV2	1051936	1464676	46.48%	6.143%
15	11.302	848	850	852	rBV	843019	702418	22.29%	2.946%
16	12.022	911	913	915	rBV	83175	116944	3.71%	0.490%
17	12.719	971	974	976	rBV	259324	211425	6.71%	0.887%
18	12.891	986	989	992	rBV	2268740	2282999	72.44%	9.575%
19	13.428	1033	1036	1037	rBV2	109669	148034	4.70%	0.621%
20	13.931	1078	1080	1083	rBV	607118	649569	20.61%	2.724%
21	15.337	1200	1203	1206	rBV	359390	523039	16.60%	2.194%

Sum of corrected areas: 23843182

LSC Report - Integrated Chromatogram

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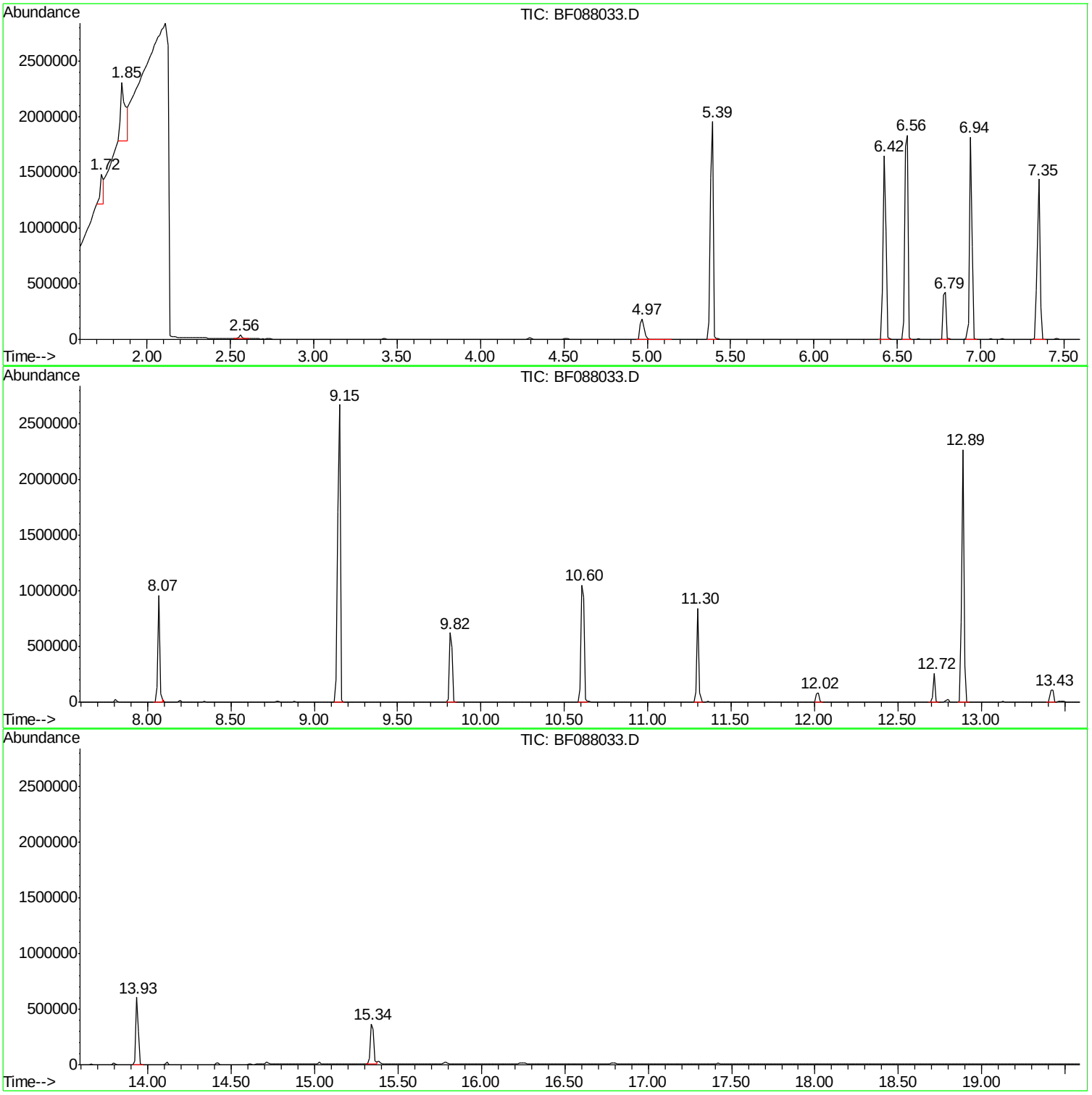
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
STA-1172-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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 : H3473-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1172-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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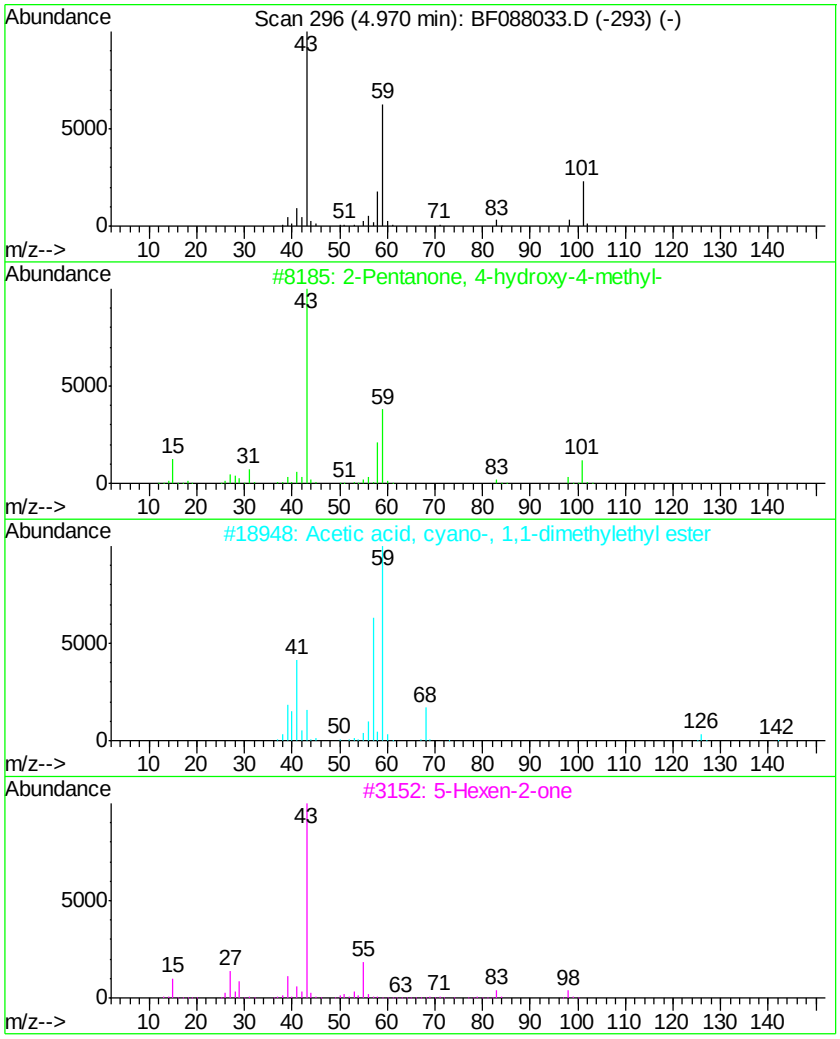
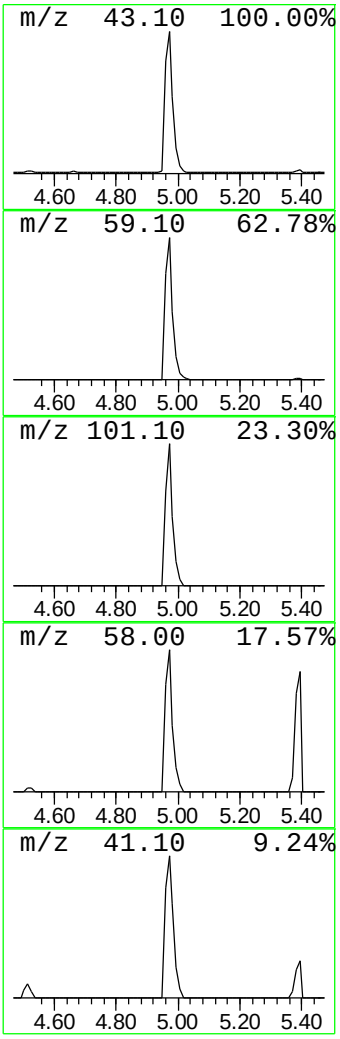
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	11.39 ng	328197	1,4-Dichlorobenzene-d4	6.79

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	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061416\
Data File : BF088033.D
Acq On : 15 Jun 2016 8:12
Operator : UM/SJ
Sample : H3473-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1172-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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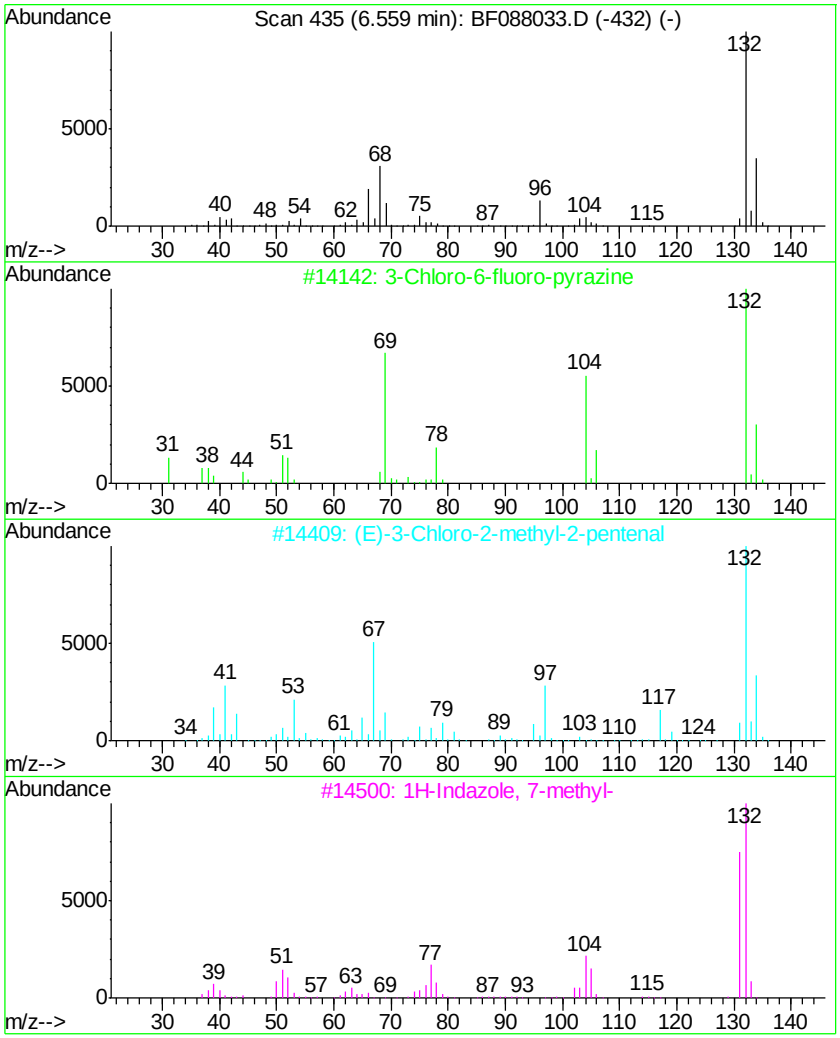
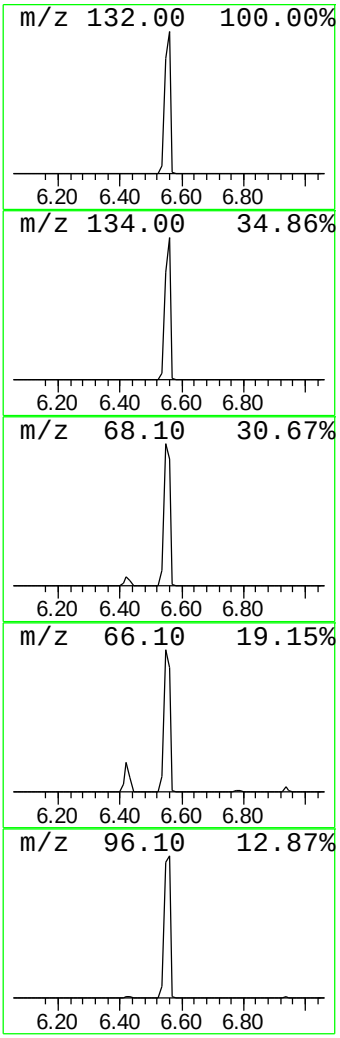
Peak Number 4 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	88.88 ng	2561640	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12
4	Amphetaminil	250	C17H18N2	017590-01-1	12
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Sample : H3473-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1172-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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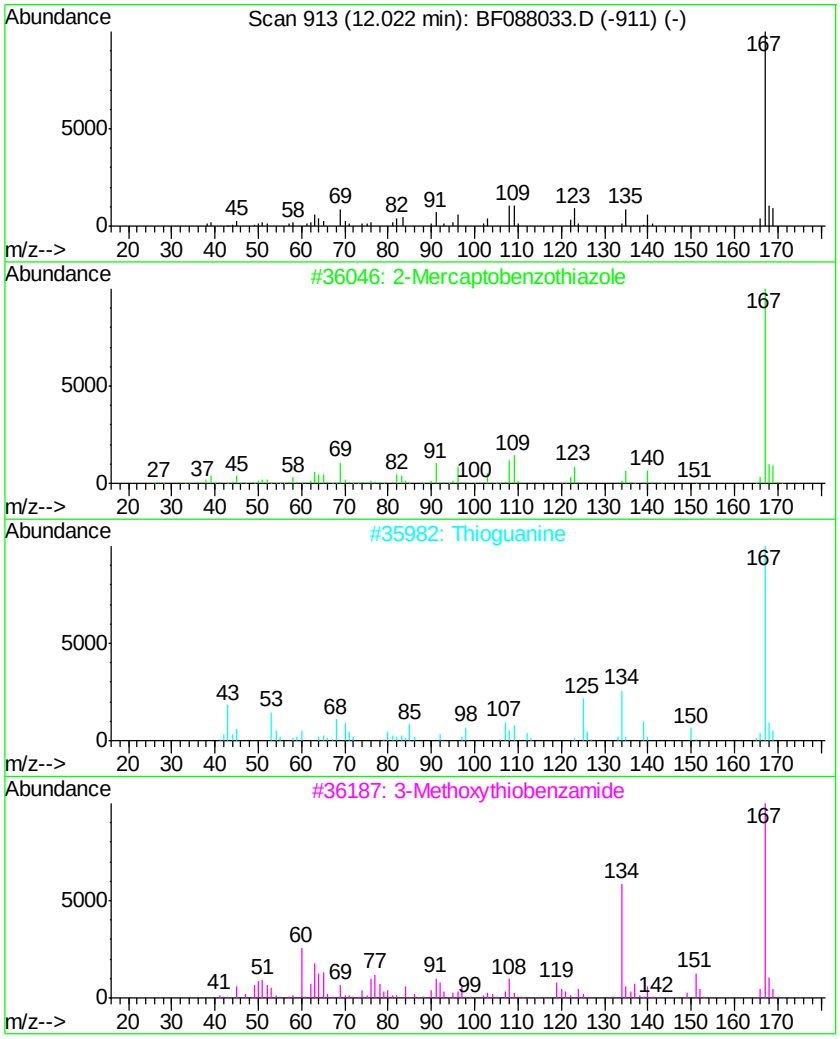
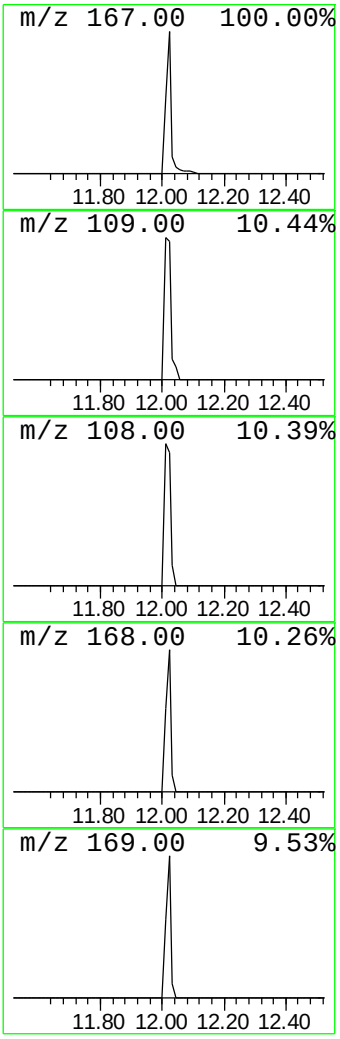
Peak Number 6 2-Mercaptobenzothiazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.33 ng	116944	Phenanthrene-d10	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2	Thioguanine	167	C5H5N5S	000154-42-7	64
3	3-Methoxythiobenzamide	167	C8H9NOS	064559-06-4	59
4	2-Methoxythiobenzamide	167	C8H9NOS	042590-97-6	53
5	2',4'-Dihydroxyacetophenone oxime	167	C8H9NO3	1000212-89-5	47





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ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1172-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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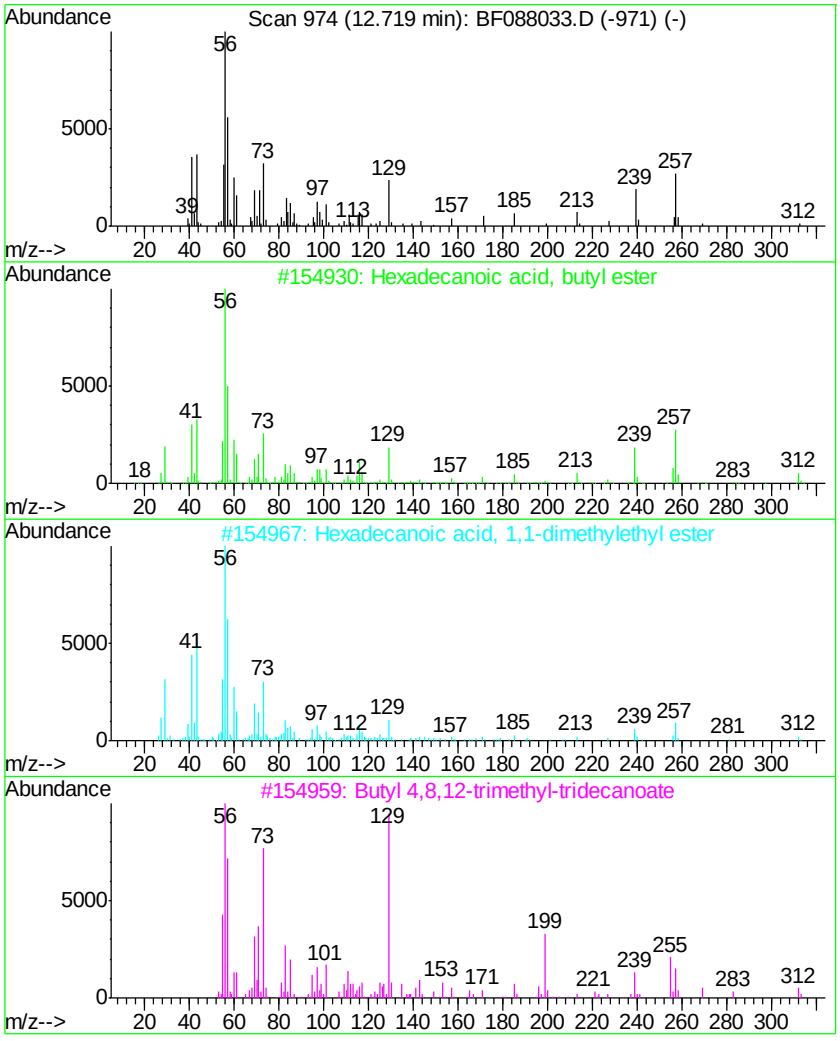
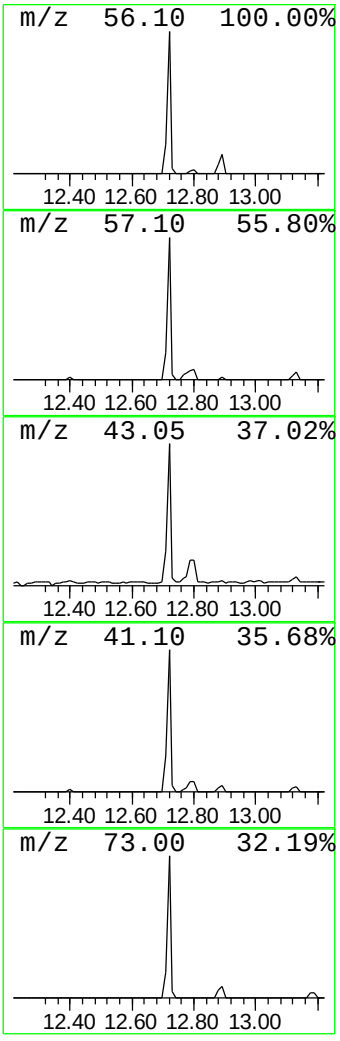
Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	6.51 ng	211425	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	45
4	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35





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Sample : H3473-19
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : STA-1172-(0-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

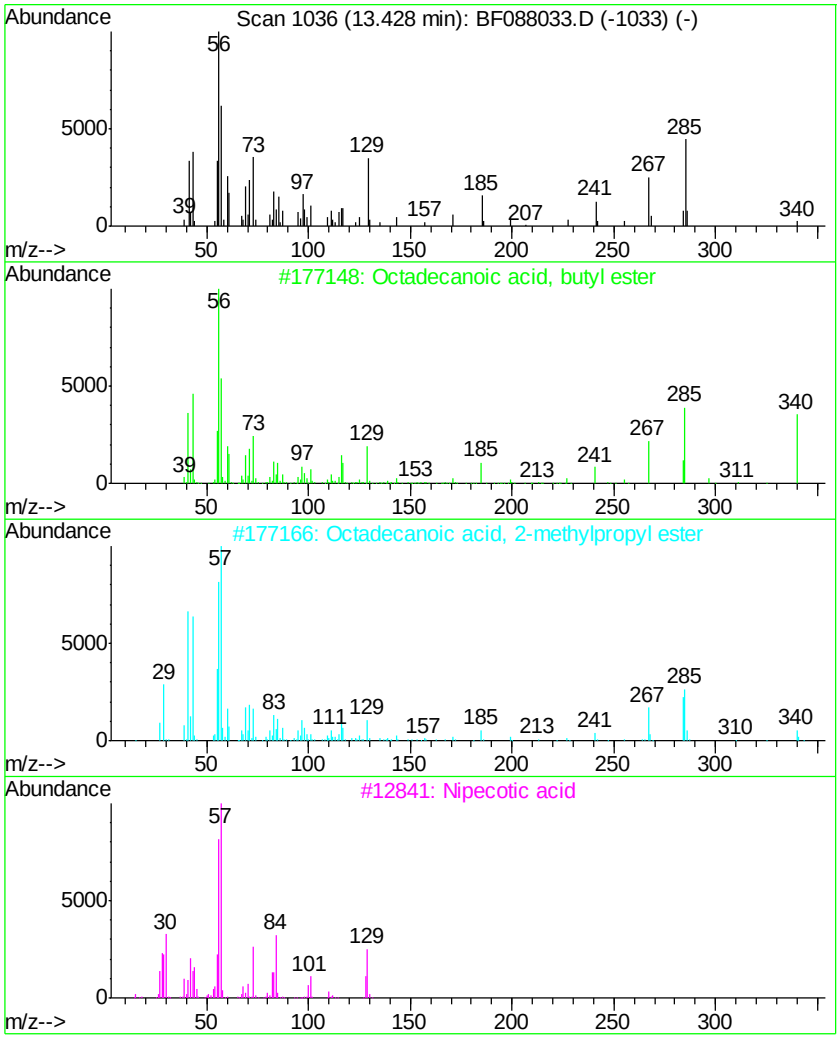
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

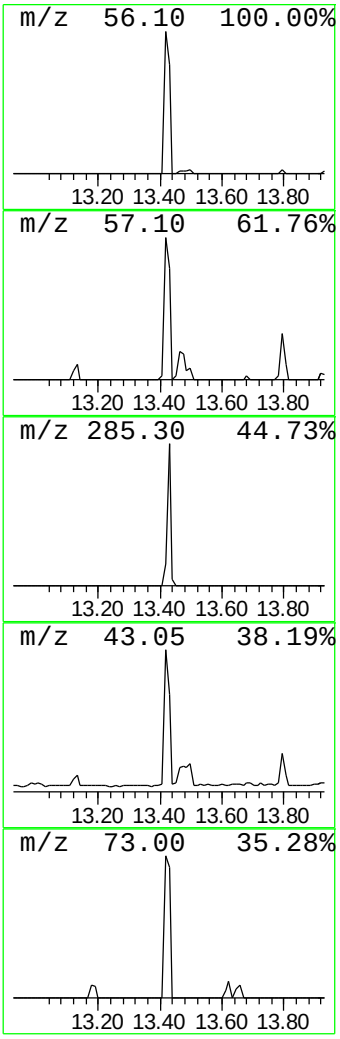
****

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	4.56 ng	148034	Chrysene-d12	13.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	86
3	Nipecotic acid	129	C6H11NO2	000498-95-3	38
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	22
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	22





Tentatively Identified Compound (LSC) summary

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ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
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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...	4.97	11.4	ng	328197	1	6.79	576439	20.0
unknown6.56	6.56	88.9	ng	2561640	1	6.79	576439	20.0
2-Mercaptobenzoth...	12.02	3.3	ng	116944	4	11.30	702418	20.0
Hexadecanoic acid...	12.72	6.5	ng	211425	5	13.93	649569	20.0
Octadecanoic acid...	13.43	4.6	ng	148034	5	13.93	649569	20.0