LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
Data File : BF098205.D
Acq On : 31 Aug 2017 20:12
Operator : SJ/JU
Sample : I4963-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3829-PA1

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-BF081517.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	4.904	475	479	489	rBV	72585	94706	2.58%	0.374%
2	5.322	541	550	553	rBV	1786915	1673049	45.63%	6.607%
3	6.351	721	725	733	rBV	1288819	1115102	30.41%	4.404%
4	6.486	743	748	751	rBV	2909646	2731513	74.49%	10.787%
5	6.716	783	787	791	rBV	906306	713200	19.45%	2.817%
6	6.875	809	814	817	rBV	2770774	2496045	68.07%	9.857%
7	7.286	878	884	887	rBV	2171760	2196604	59.90%	8.675%
8	7.998	1001	1005	1009	rBV	1085626	957897	26.12%	3.783%
9	8.280	1048	1053	1058	rBV	736643	720350	19.64%	2.845%
10	9.080	1183	1189	1192	rBV	3740114	3666882	100.00%	14.481%
11	9.192	1203	1208	1213	rVB5	26986	49023	1.34%	0.194%
12	9.751	1299	1303	1307	rBV2	1161258	1018433	27.77%	4.022%
13	10.380	1407	1410	1414	rVB	46545	44765	1.22%	0.177%
14	10.539	1432	1437	1441	rBV	1844209	1994385	54.39%	7.876%
15	10.657	1452	1457	1466	rVB	238436	272137	7.42%	1.075%
16	11.233	1551	1555	1558	rBV	1133457	937619	25.57%	3.703%
17	11.774	1644	1647	1650	rBV	170625	155064	4.23%	0.612%
18	11.957	1675	1678	1685	rBV	179946	193834	5.29%	0.765%
19	12.563	1778	1781	1785	rBV	251481	247304	6.74%	0.977%
20	12.821	1821	1825	1829	rBV	2537833	2748585	74.96%	10.855%
21	13.868	2000	2003	2007	rVB	717629	631165	17.21%	2.493%
22	15.286	2240	2244	2254	rVB	492460	664018	18.11%	2.622%

Sum of corrected areas: 25321680

LSC Report - Integrated Chromatogram

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Misc :
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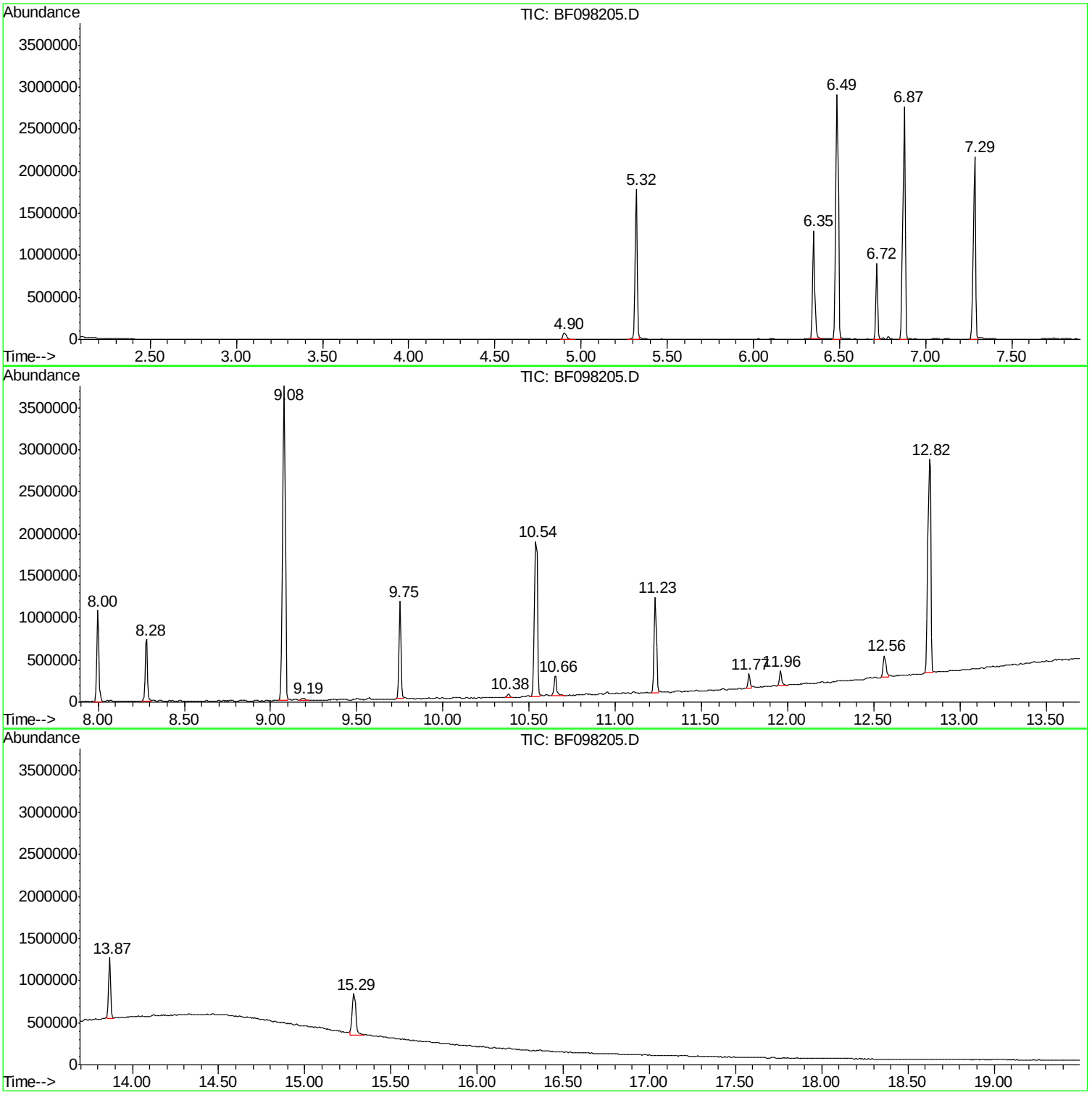
Instrument : BNA_F
ClientSampleId : 3829-PA1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
Data File : BF098205.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

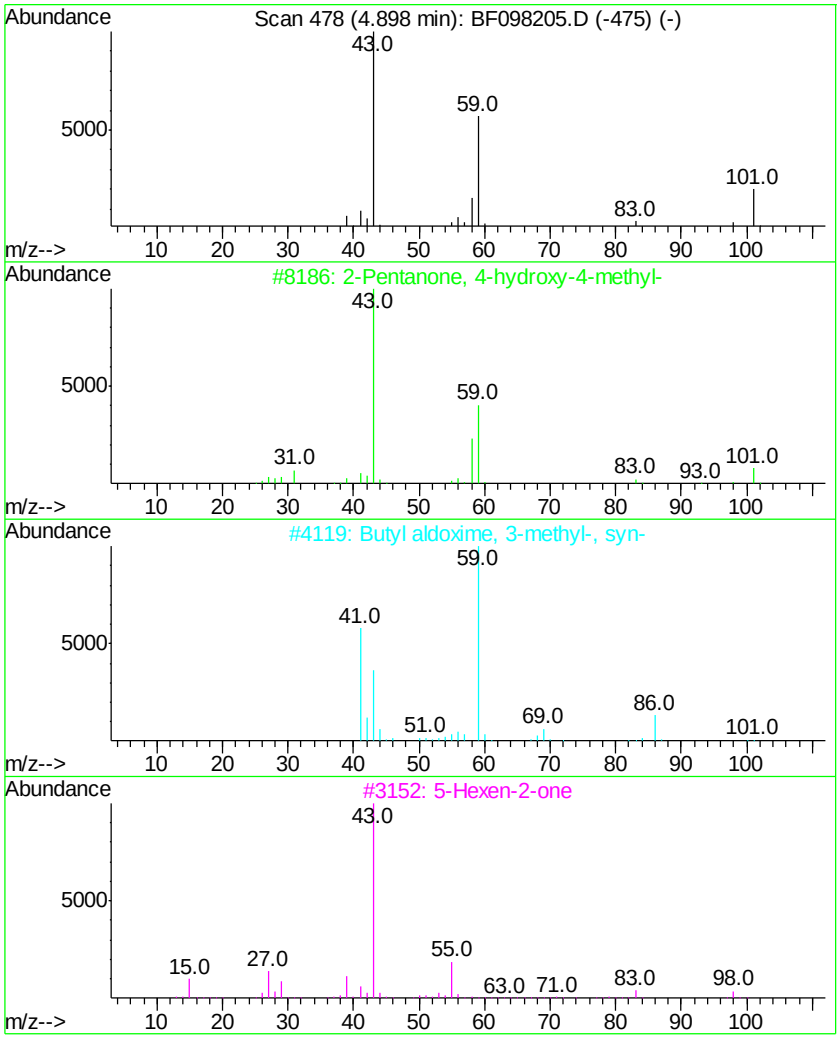
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

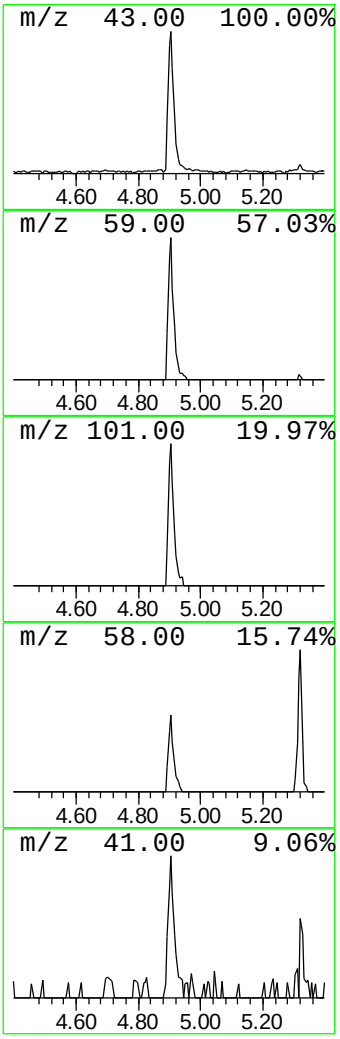
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.66 ng	94706	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	10
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





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Sample : I4963-10
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Instrument : BNA_F
ClientSampleId : 3829-PA1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

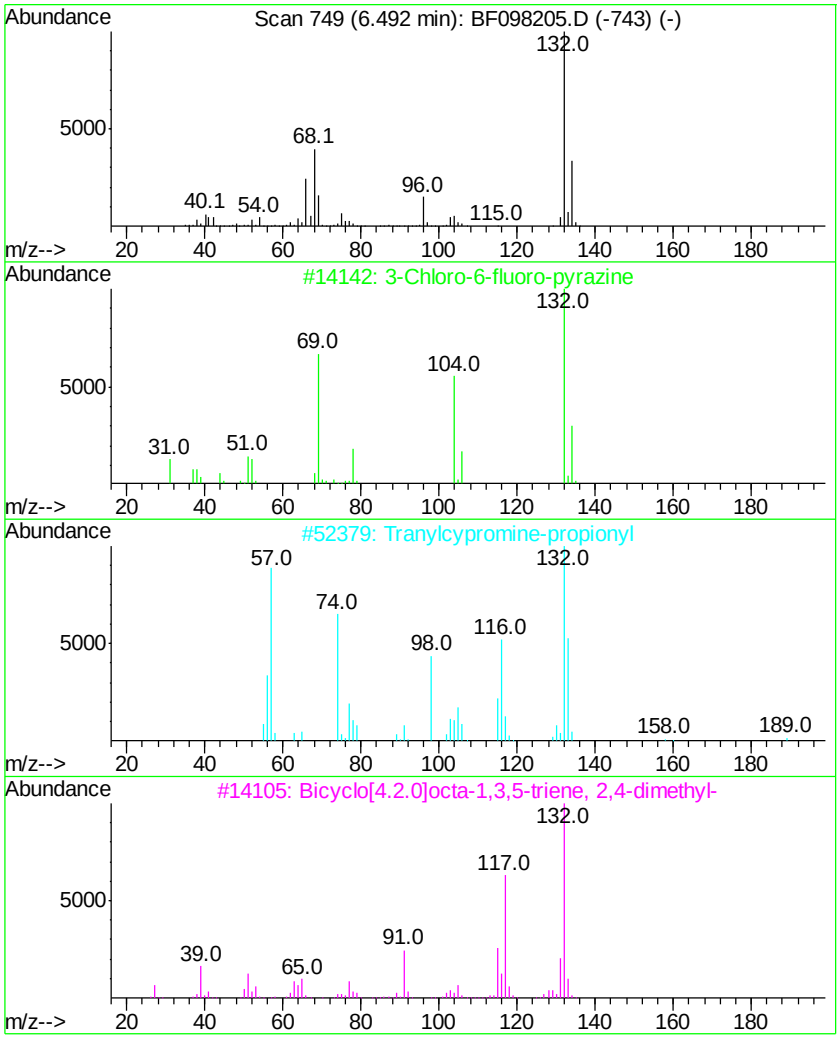
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

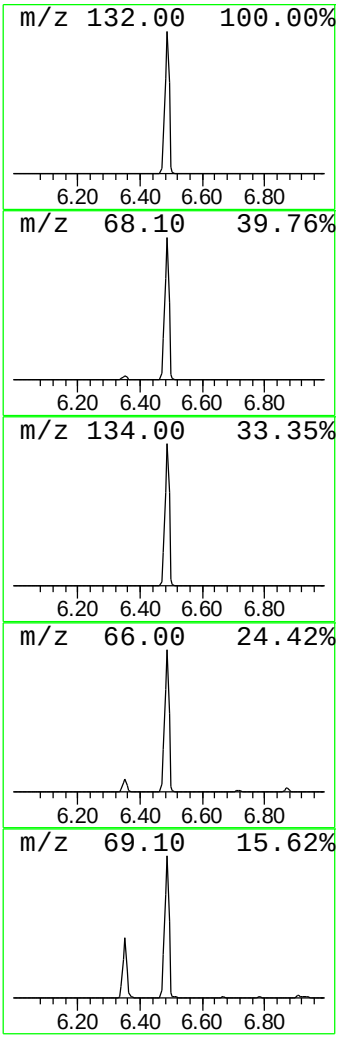
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	76.60 ng	2731510	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Data File : BF098205.D
Acq On : 31 Aug 2017 20:12
Operator : SJ/JU
Sample : I4963-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3829-PA1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

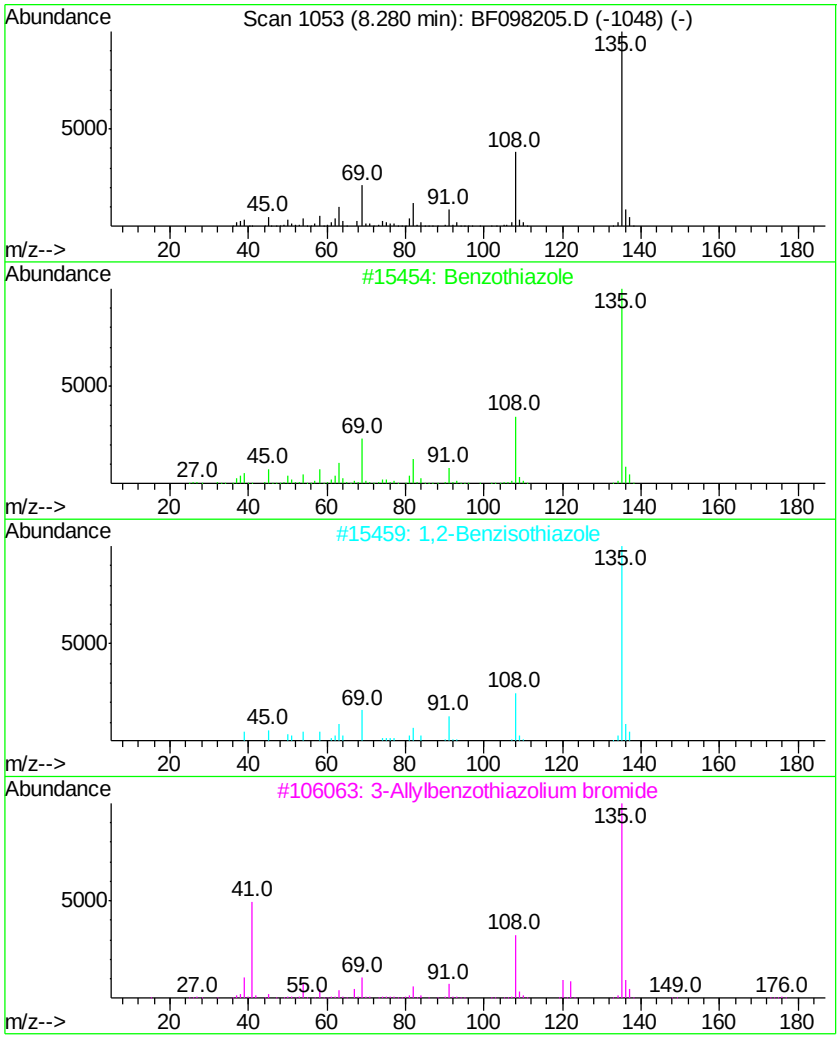
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

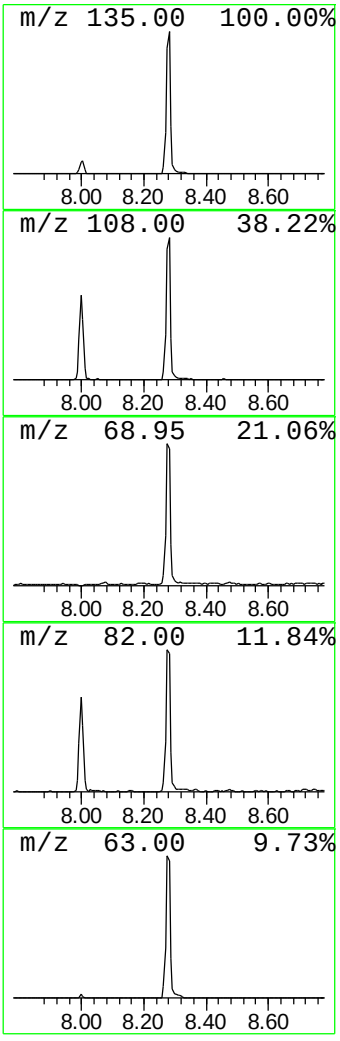
****

Peak Number 4 Benzothiazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	15.04 ng	720350	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	97
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	83
3	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	78
4	2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	72
5	Adenine	135	C5H5N5	000073-24-5	64





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Data File : BF098205.D
Acq On : 31 Aug 2017 20:12
Operator : SJ/JU
Sample : I4963-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3829-PA1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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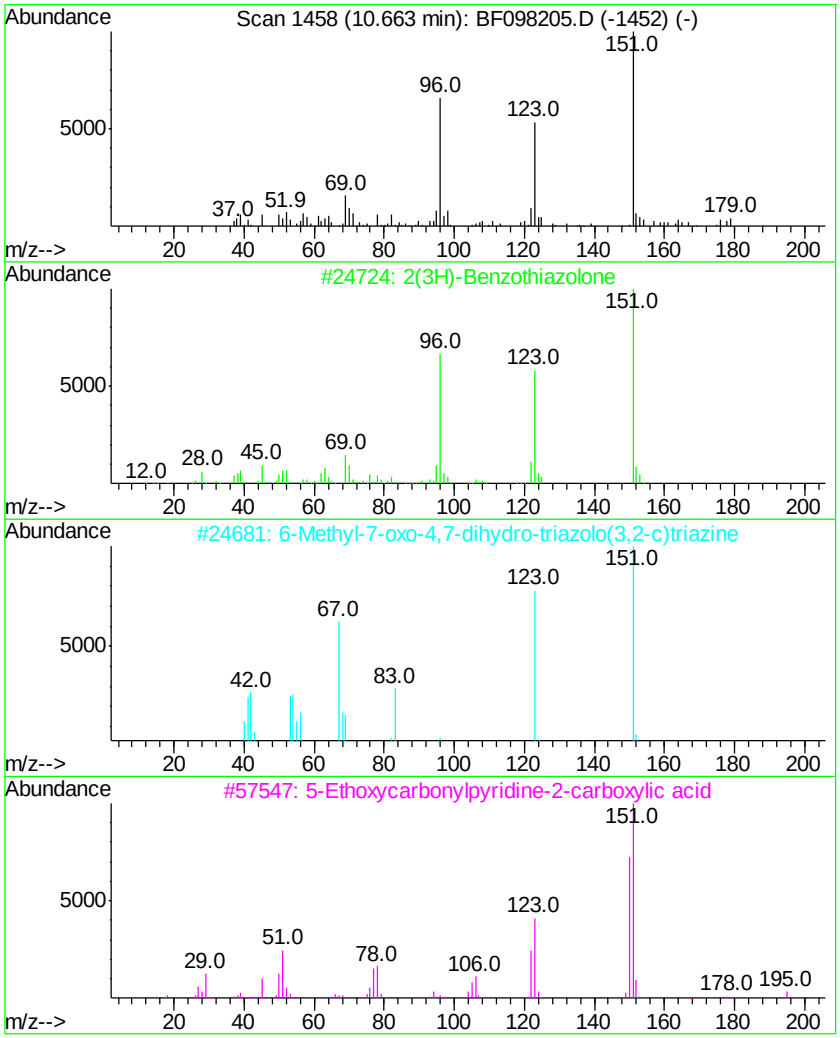
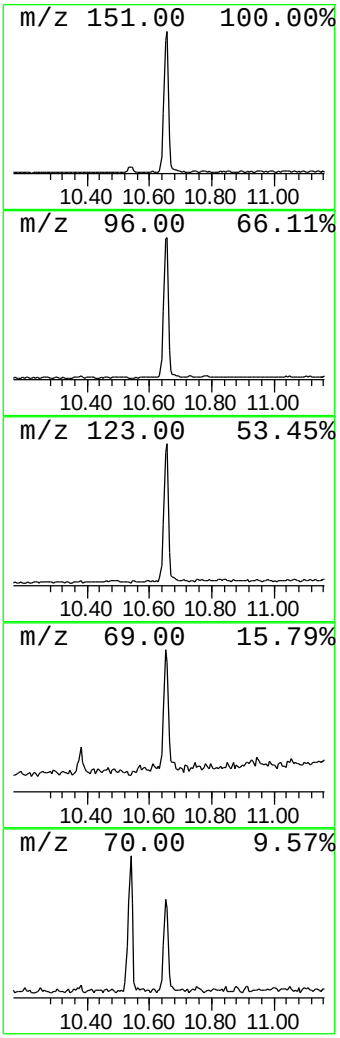
Peak Number 5 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	5.80 ng	272137	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
2	6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	43
3	5-Ethoxycarbonylpyridine-2-carbo...	195	C9H9NO4	017880-34-1	37
4	2,4-Dioxabicyclo[4.4.0]decan-5-o...	212	C12H20O3	124899-16-7	37
5	4-Methoxyformanilide	151	C8H9NO2	005470-34-8	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF083117\
Data File : BF098205.D
Acq On : 31 Aug 2017 20:12
Operator : SJ/JU
Sample : I4963-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3829-PA1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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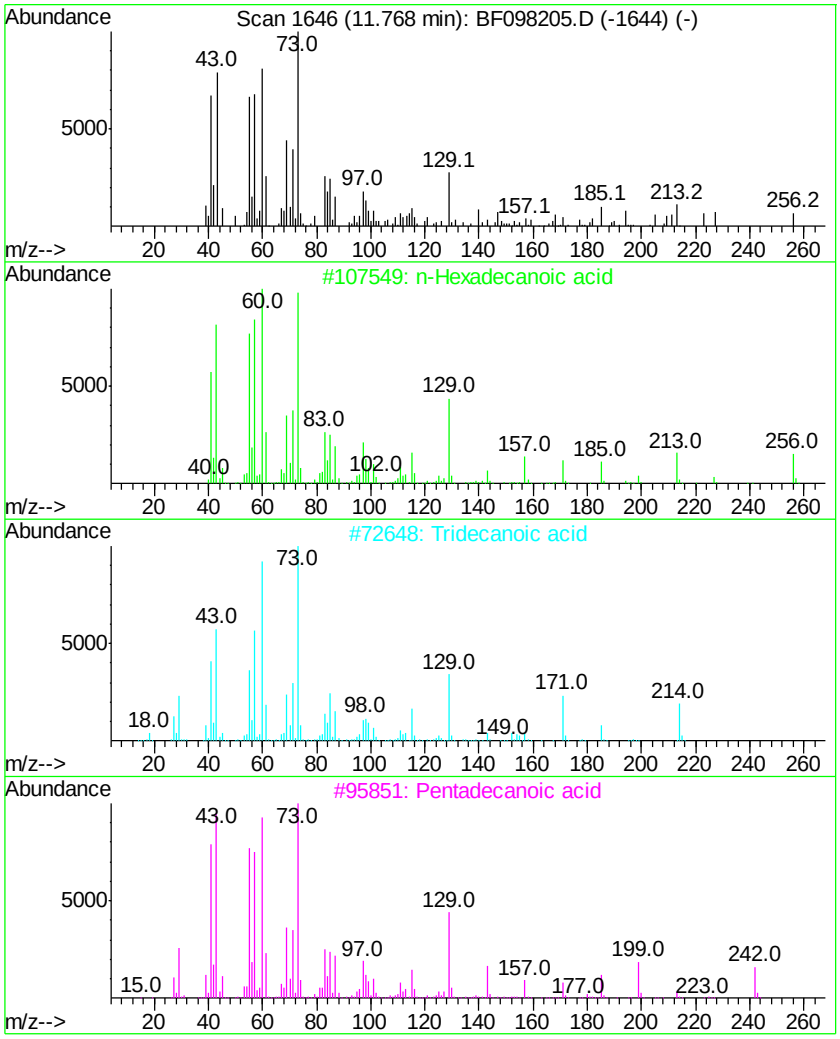
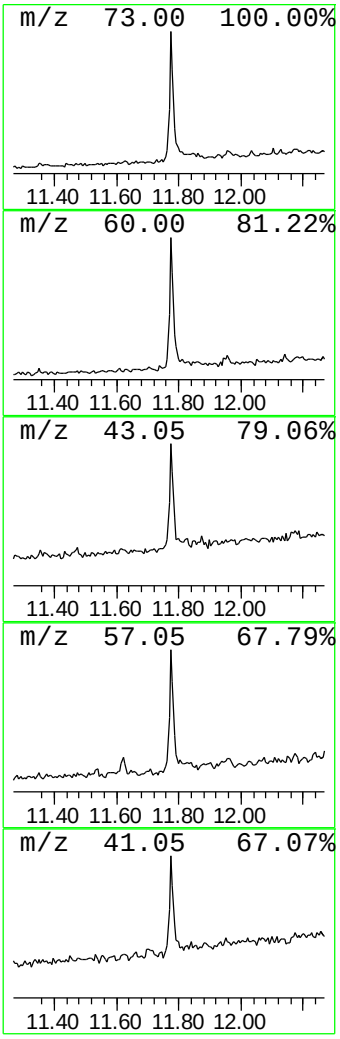
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	3.31 ng	155064	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25





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Misc :
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Instrument : BNA_F
ClientSampleId : 3829-PA1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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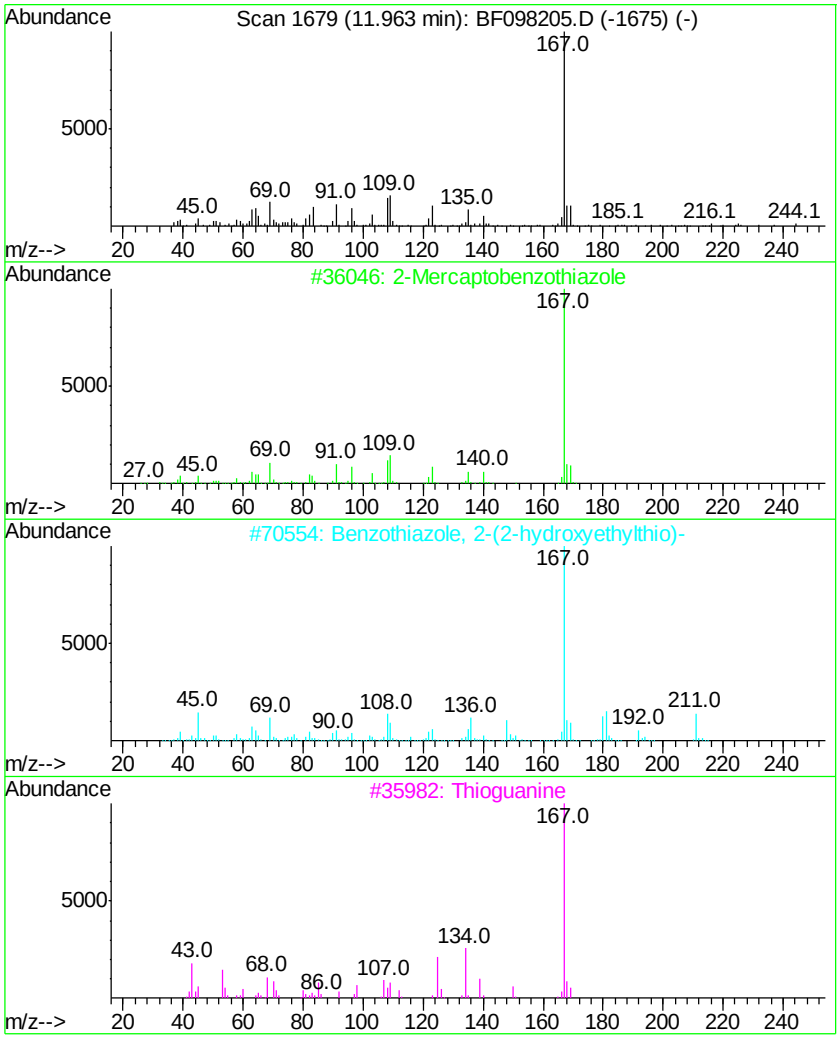
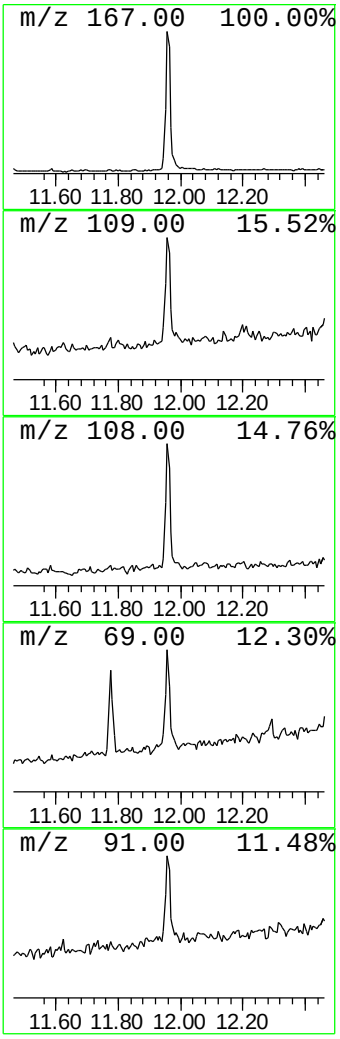
Peak Number 7 2-Mercaptobenzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	4.13 ng	193834	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	97
2	Benzothiazole, 2-(2-hydroxyethyl...	211	C9H9NOS2	004665-63-8	64
3	Thioguanine	167	C5H5N5S	000154-42-7	53
4	Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	50
5	6H-Purine-6-thione, 9-amino-1,9-...	167	C5H5N5S	020914-56-1	47





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

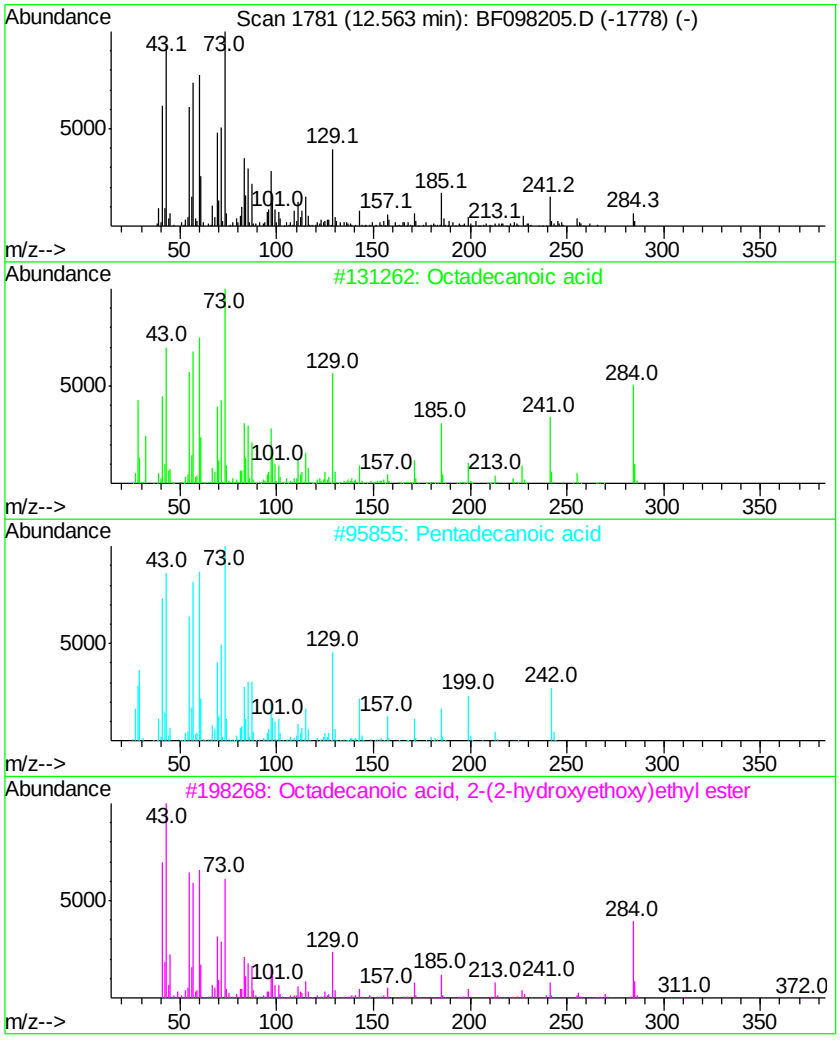
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

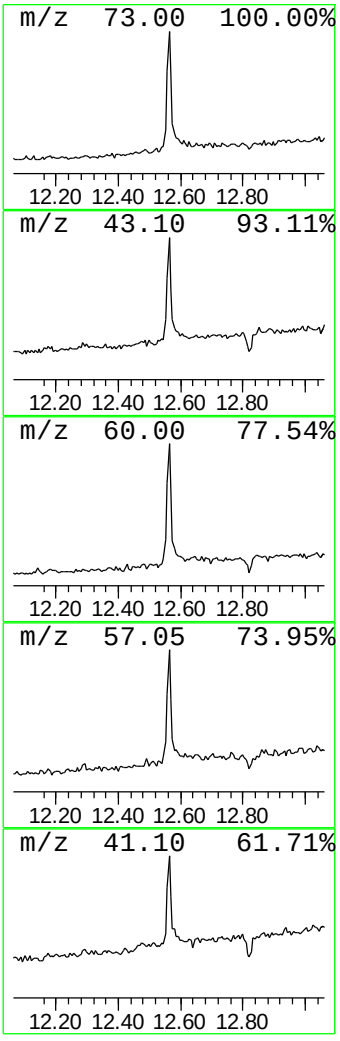
****

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	7.84 ng	247304	Chrysene-d12	13.87

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	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	2.7	ng	94706	1	6.72	713200	20.0
unknown6.49	6.49	76.6	ng	2731510	1	6.72	713200	20.0
Benzothiazole	8.28	15.0	ng	720350	2	8.00	957897	20.0
2(3H)-Benzothiazo...	10.66	5.8	ng	272137	4	11.23	937619	20.0
n-Hexadecanoic acid	11.77	3.3	ng	155064	4	11.23	937619	20.0
2-Mercaptobenzoth...	11.96	4.1	ng	193834	4	11.23	937619	20.0
Octadecanoic acid	12.56	7.8	ng	247304	5	13.87	631165	20.0