LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082200.D
Acq On : 11 Oct 2015 3:11
Operator : UM/IZ
Sample : G3959-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PO-002

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-BF101015.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	2.331	14	17	32	rVB3	14860	53145	1.65%	0.233%
2	4.480	202	205	208	rBV	86792	106124	3.30%	0.466%
3	5.006	249	251	261	rVB	307108	396547	12.31%	1.740%
4	5.429	286	288	291	rBV	1232073	1154270	35.84%	5.066%
5	6.469	376	379	381	rBV	741232	762922	23.69%	3.348%
6	6.606	388	391	393	rBV	2072309	2187675	67.93%	9.601%
7	6.834	409	411	414	rBV	582780	526723	16.35%	2.312%
8	6.994	422	425	427	rBV	2088735	2106264	65.40%	9.244%
9	7.406	458	461	464	rBV	1290095	1460430	45.35%	6.410%
10	8.126	521	524	526	rBV	665463	689916	21.42%	3.028%
11	9.200	615	618	621	rBV	2488501	3077536	95.56%	13.507%
12	9.600	650	653	654	rBV	144195	144164	4.48%	0.633%
13	9.875	675	677	680	rBV	743934	820685	25.48%	3.602%
14	10.526	732	734	740	rBV2	51762	66556	2.07%	0.292%
15	10.675	744	747	749	rBV	1647592	1981389	61.52%	8.696%
16	10.732	749	752	755	rVV	103541	173518	5.39%	0.762%
17	10.778	755	756	758	rVV	46132	51637	1.60%	0.227%
18	10.823	758	760	763	rVB	63740	66598	2.07%	0.292%
19	11.223	793	795	797	rBV	35304	37375	1.16%	0.164%
20	11.361	805	807	810	rBV	718536	809389	25.13%	3.552%
21	11.898	851	854	856	rBV	100174	112149	3.48%	0.492%
22	11.966	856	860	862	rVB	257675	350897	10.90%	1.540%
23	12.572	911	913	914	rBV	25685	33097	1.03%	0.145%
24	12.675	920	922	926	rBV3	27280	42620	1.32%	0.187%
25	12.766	929	930	936	rBV3	21802	34292	1.06%	0.151%
26	12.961	944	947	949	rBV	2437262	3220635	100.00%	14.135%
27	13.441	986	989	991	rBV	57307	55645	1.73%	0.244%
28	13.509	993	995	997	rVV2	17674	33092	1.03%	0.145%
29	13.555	997	999	1004	rVB2	38313	80209	2.49%	0.352%
30	13.852	1023	1025	1032	rVB	78565	133738	4.15%	0.587%
31	14.001	1036	1038	1041	rVV	747968	724399	22.49%	3.179%
32	14.424	1070	1075	1078	rBV	37238	81061	2.52%	0.356%
33	15.292	1148	1151	1154	rBV3	18713	35698	1.11%	0.157%
34	15.441	1161	1164	1171	rBV	399189	603841	18.75%	2.650%

LSC Area Percent Report

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Misc :
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Instrument :
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ClientSampleId :
PO-002

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-BF101015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.830	1196	1198	1200	rBV2	18660	38398	1.19%	0.169%
36	15.932	1203	1207	1210	rVV3	21184	55536	1.72%	0.244%
37	15.990	1210	1212	1217	rVB	19370	33381	1.04%	0.147%
38	16.104	1219	1222	1229	rBV	157795	278136	8.64%	1.221%
39	16.481	1252	1255	1261	rVB4	12764	38369	1.19%	0.168%
40	16.618	1264	1267	1273	rVB	62299	126954	3.94%	0.557%

Sum of corrected areas: 22785010

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Instrument :
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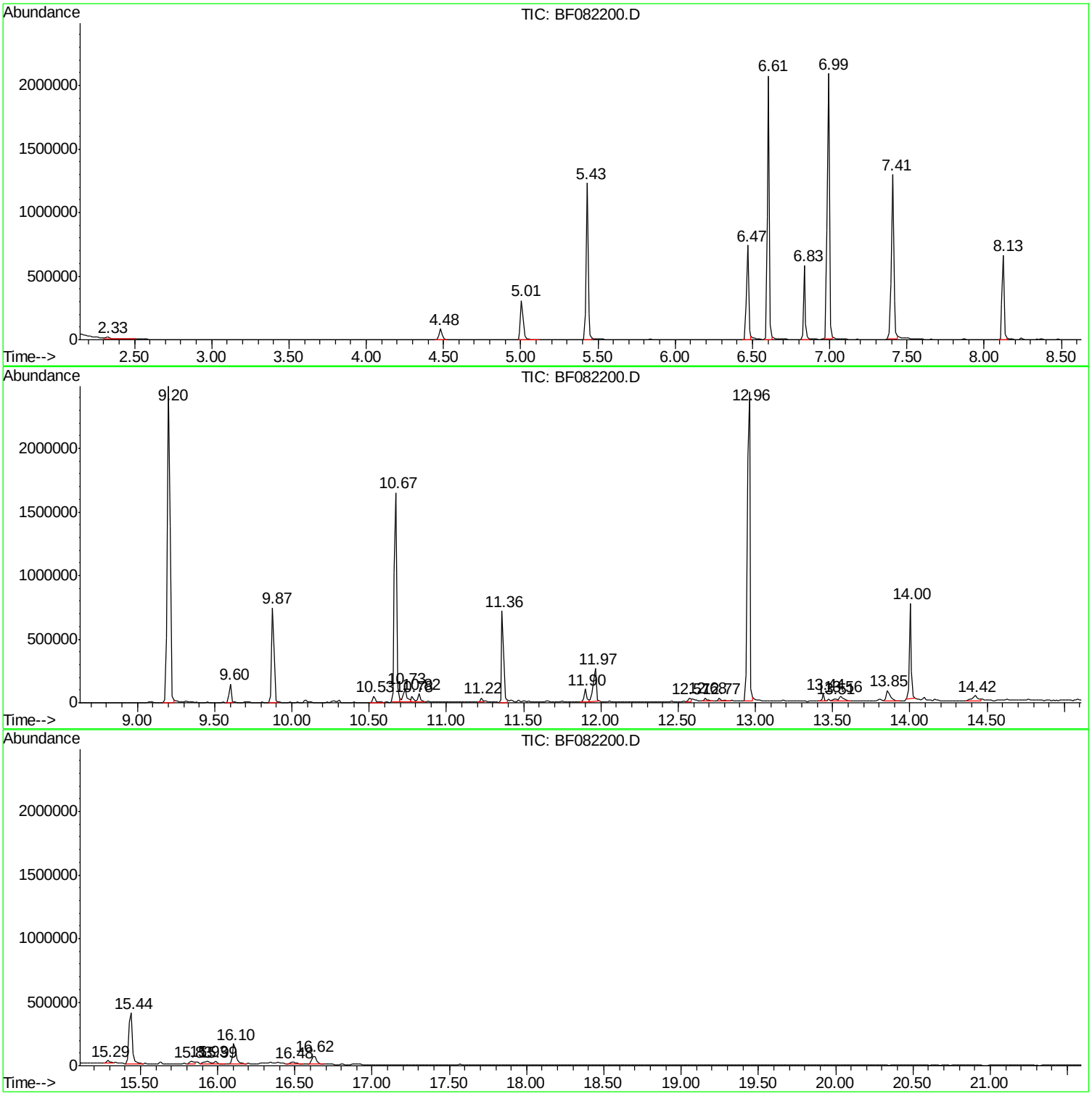
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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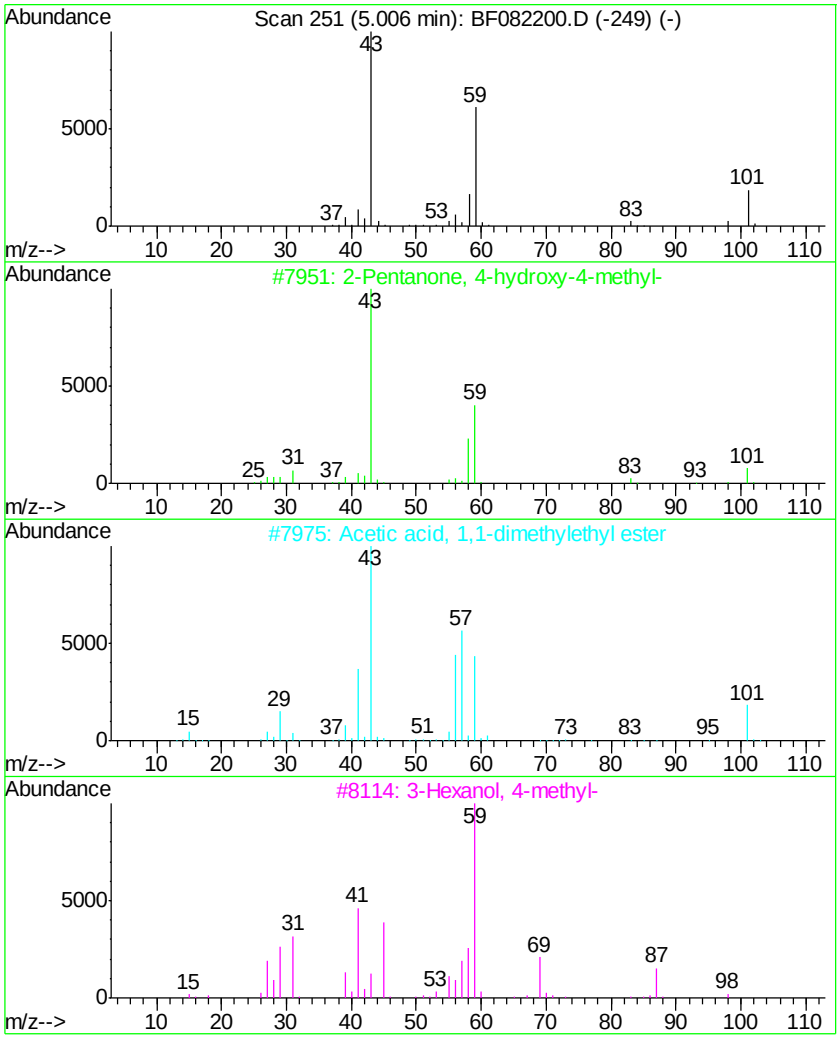
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

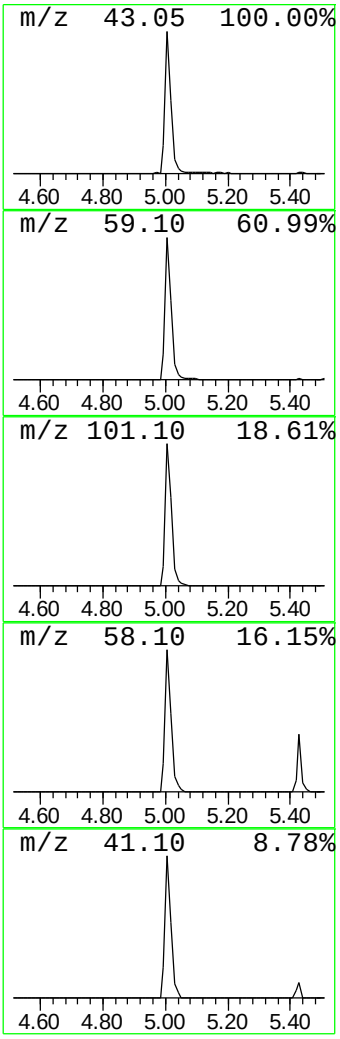
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	15.06 ng	396547	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Sample : G3959-04
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ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
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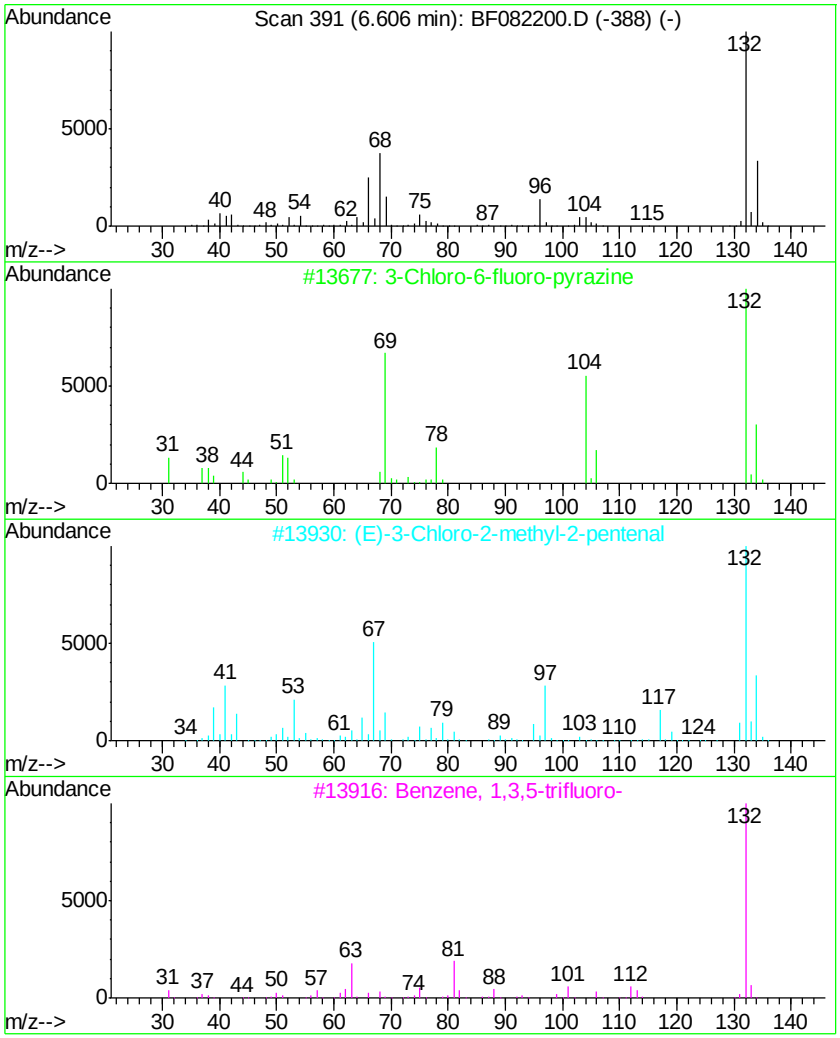
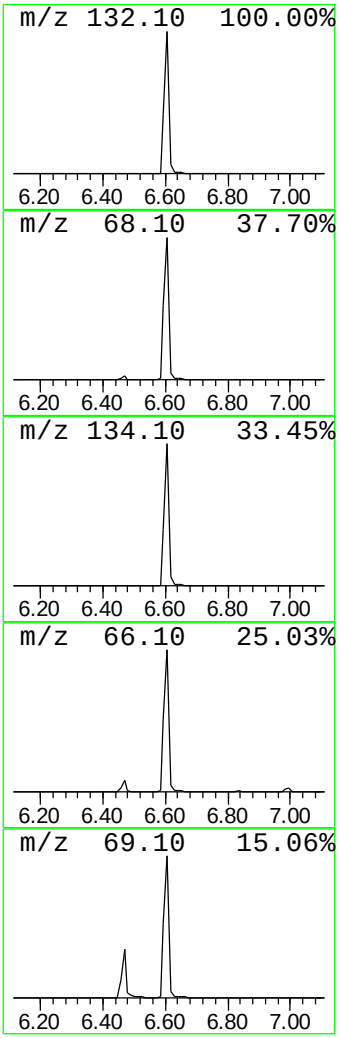
****

Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	83.07 ng	2187680	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Instrument :
BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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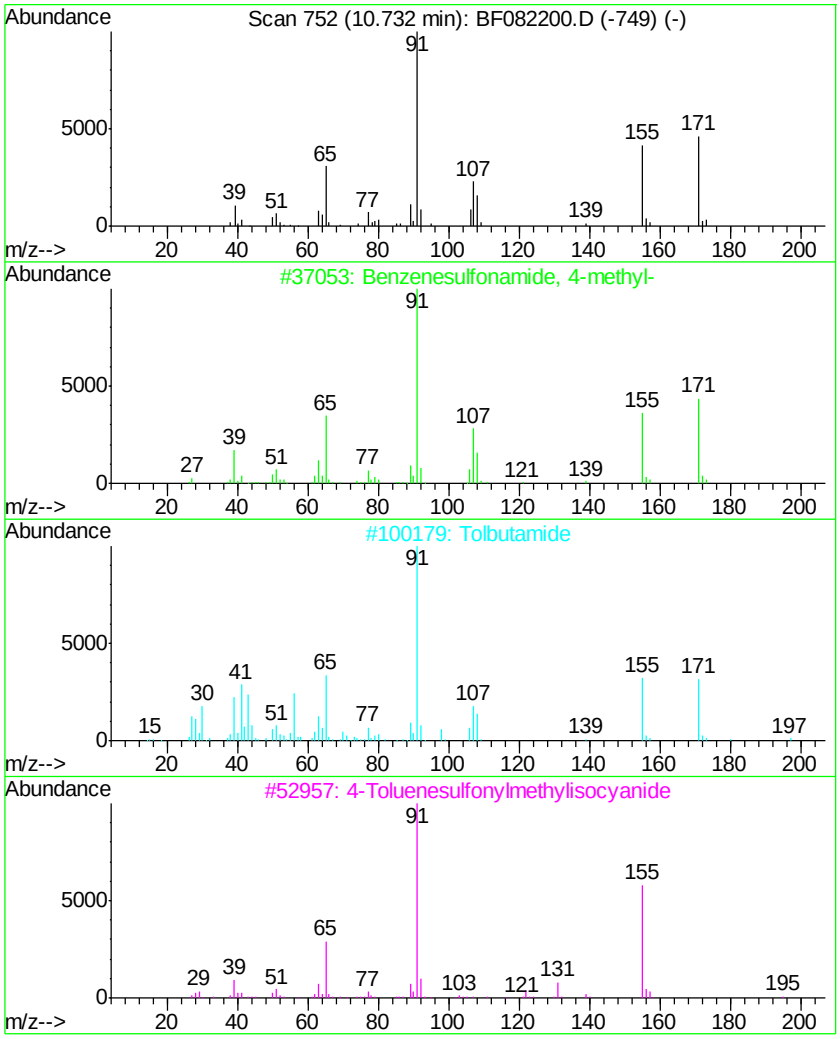
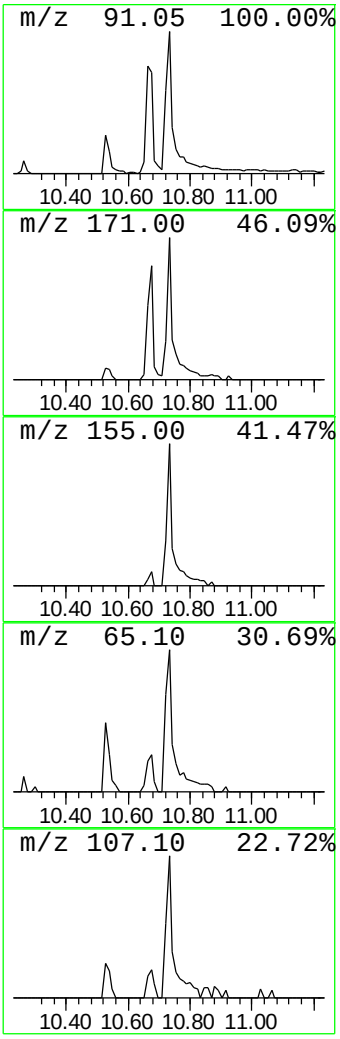
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzenesulfonamide, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	4.29 ng	173518	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	95
2	Tolbutamide	270	C12H18N2O3S	000064-77-7	47
3	4-Toluenesulfonylmethylisocyanide	195	C9H9NO2S	036635-61-7	46
4	Thiophene-3-ol, 2,3-dihydro-, 4-...	288	C11H12O5S2	039582-96-2	38
5	Benzenesulfonamide, N,4-dimethyl...	214	C8H10N2O3S	000080-11-5	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
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Sample : G3959-04
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ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

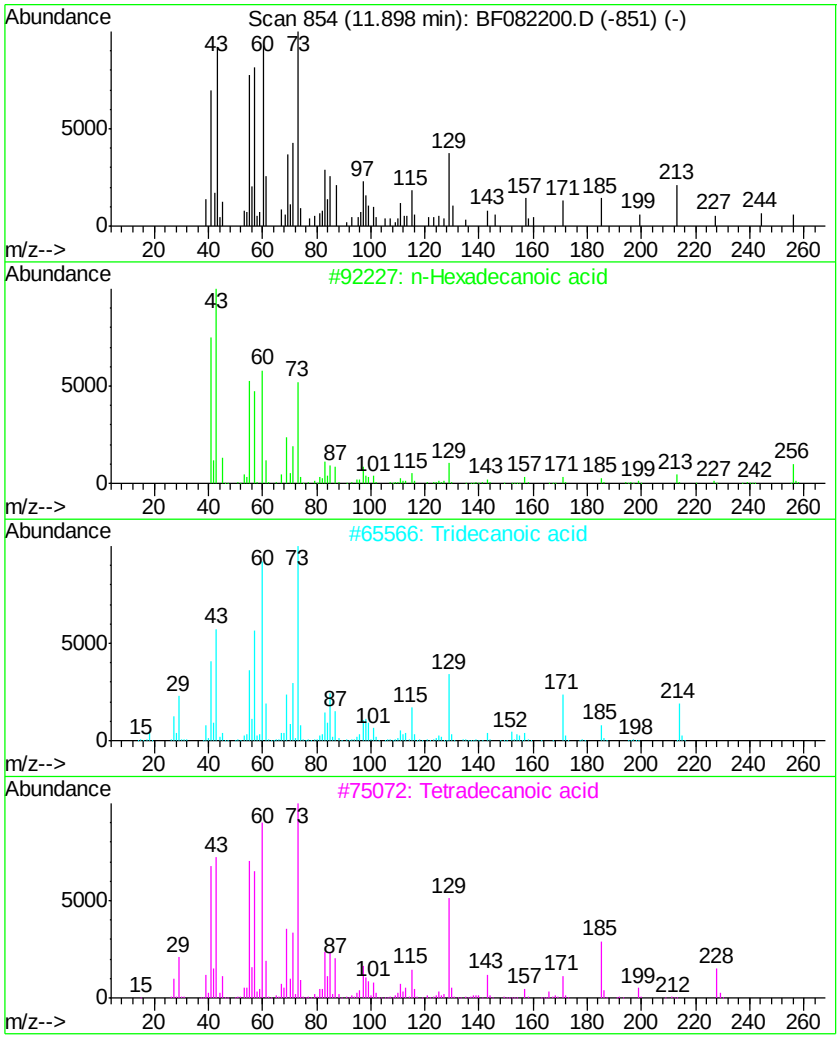
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

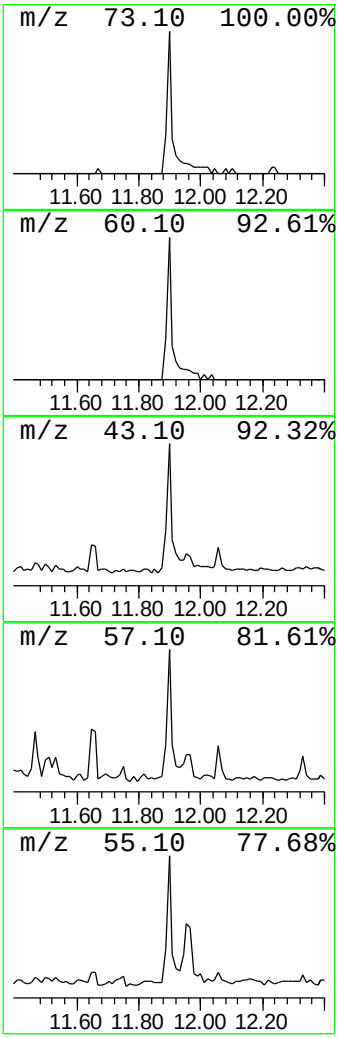
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.77 ng	112149	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5	Nonanoic acid	158	C9H18O2	000112-05-0	27





Library Search Compound Report

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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

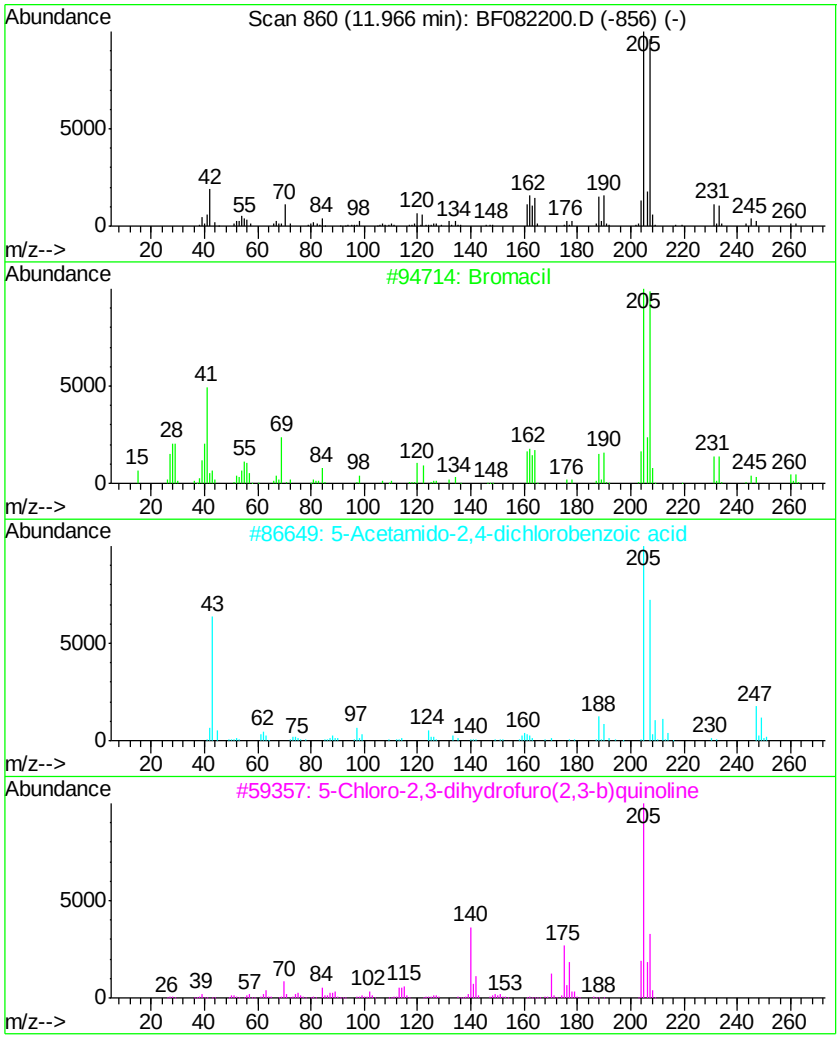
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

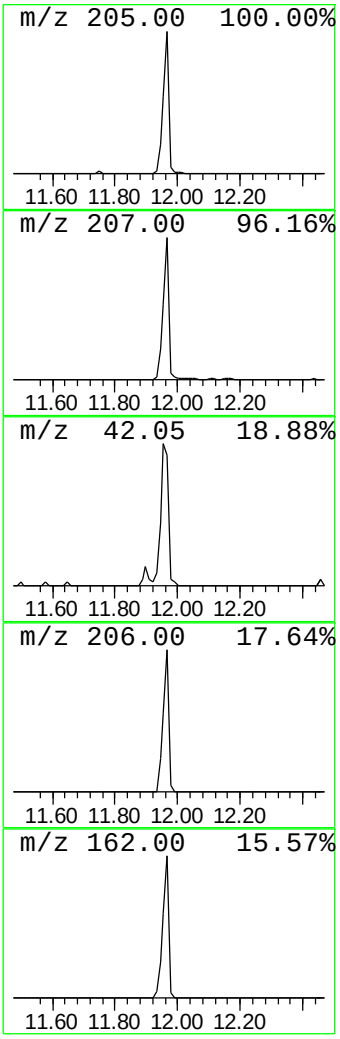
****

Peak Number 8 Bromacil Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	8.67 ng	350897	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromacil	260	C9H13BrN2O2	000314-40-9	91
2	5-Acetamido-2,4-dichlorobenzoic ...	247	C9H7Cl2NO3	050602-49-8	64
3	5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	43
4	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	42
5	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	40





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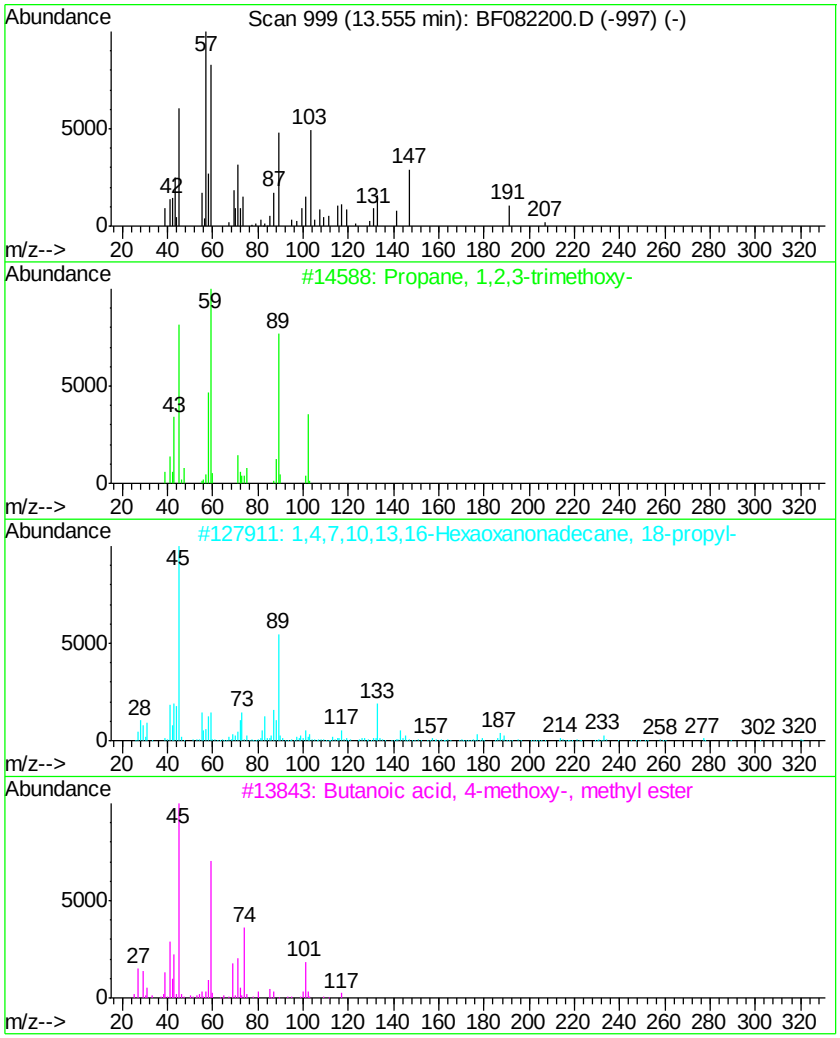
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

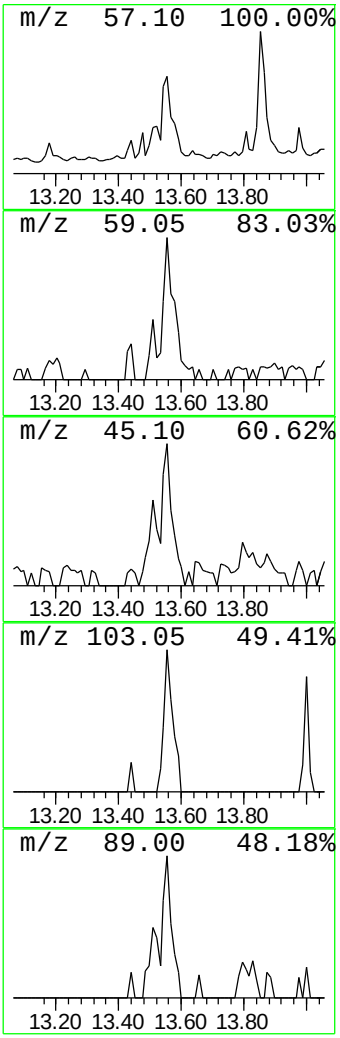
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 unknown13.56 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	2.21 ng	80209	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,2,3-trimethoxy-	134	C6H14O3	020637-49-4	38
2	1,4,7,10,13,16-Hexaoxanonadecane...	320	C16H32O6	1000163-65-3	27
3	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	25
4	3-Hexanol, 1,5-dimethoxy-2,4-dim...	190	C10H22O3	013897-22-8	25
5	Butanoic acid, 4-ethoxy-, methyl...	146	C7H14O3	029006-04-0	25





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TIC Library : C:\DATABASE\NIST02.L
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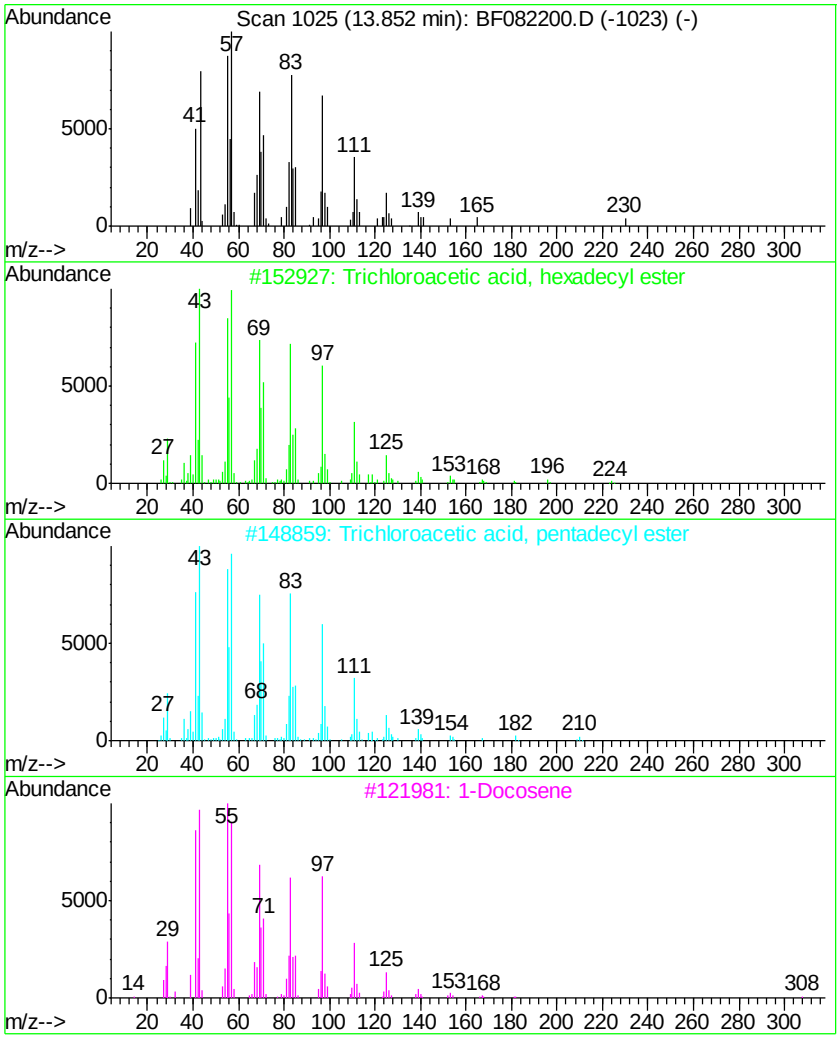
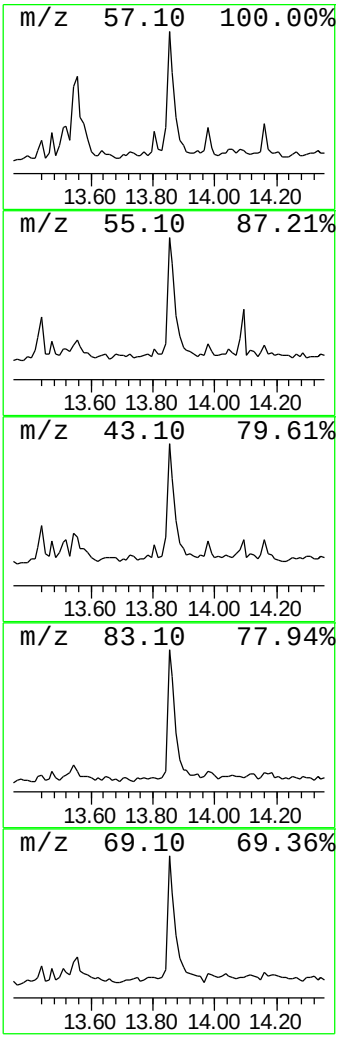
****
Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.69 ng	133738	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
3	1-Docosene	308	C22H44	001599-67-3	94
4	Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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BNA_F
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PO-002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

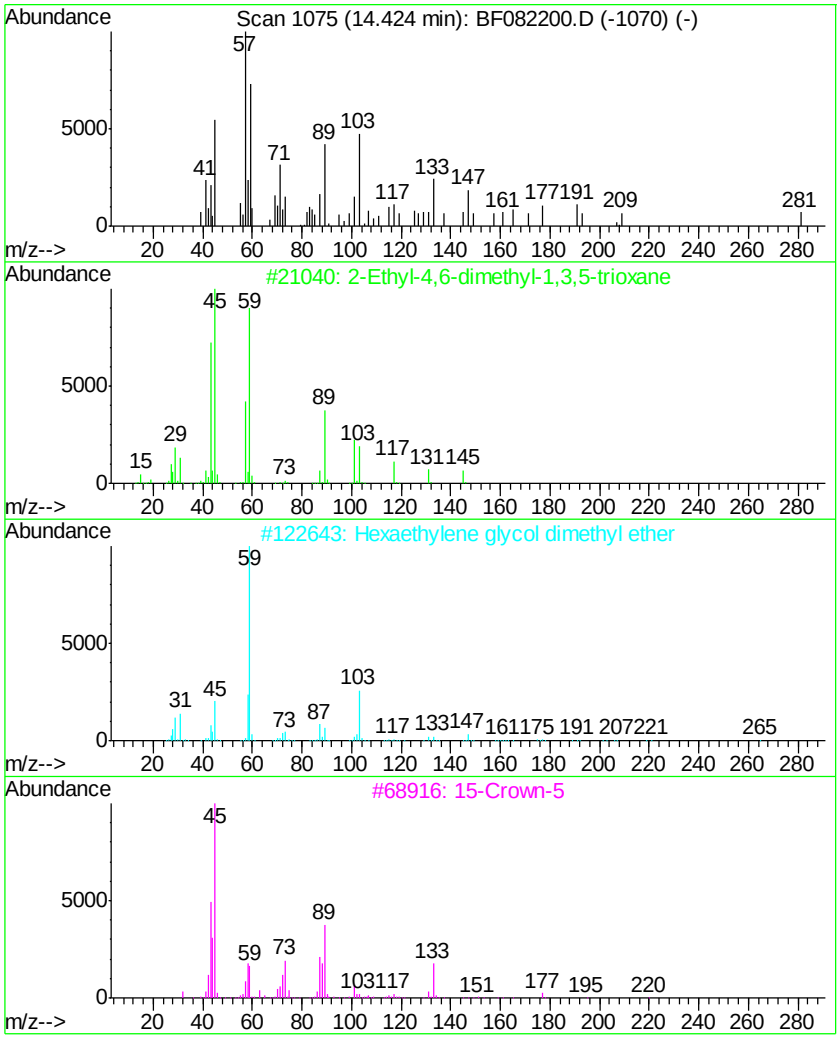
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

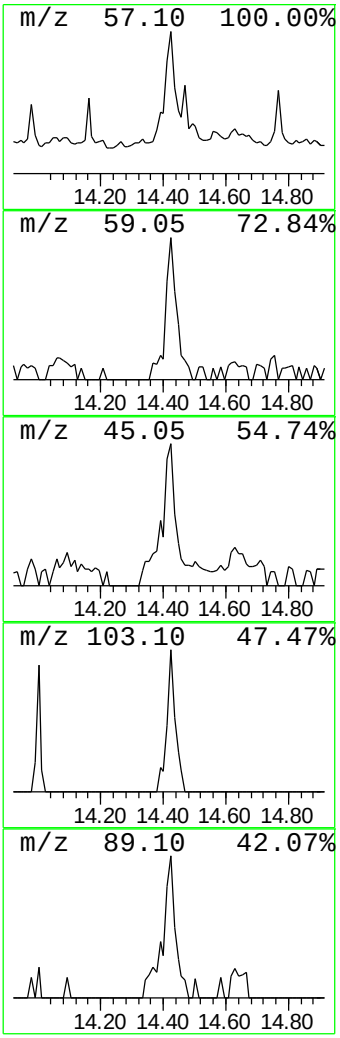
****

Peak Number 11 unknown14.42 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	2.24 ng	81061	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-4,6-dimethyl-1,3,5-trioxane	146	C7H14O3	024261-86-7	38
2	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	35
3	15-Crown-5	220	C10H20O5	033100-27-5	32
4	Propane, 1,2,3-trimethoxy-	134	C6H14O3	020637-49-4	32
5	Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	27





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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PO-002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

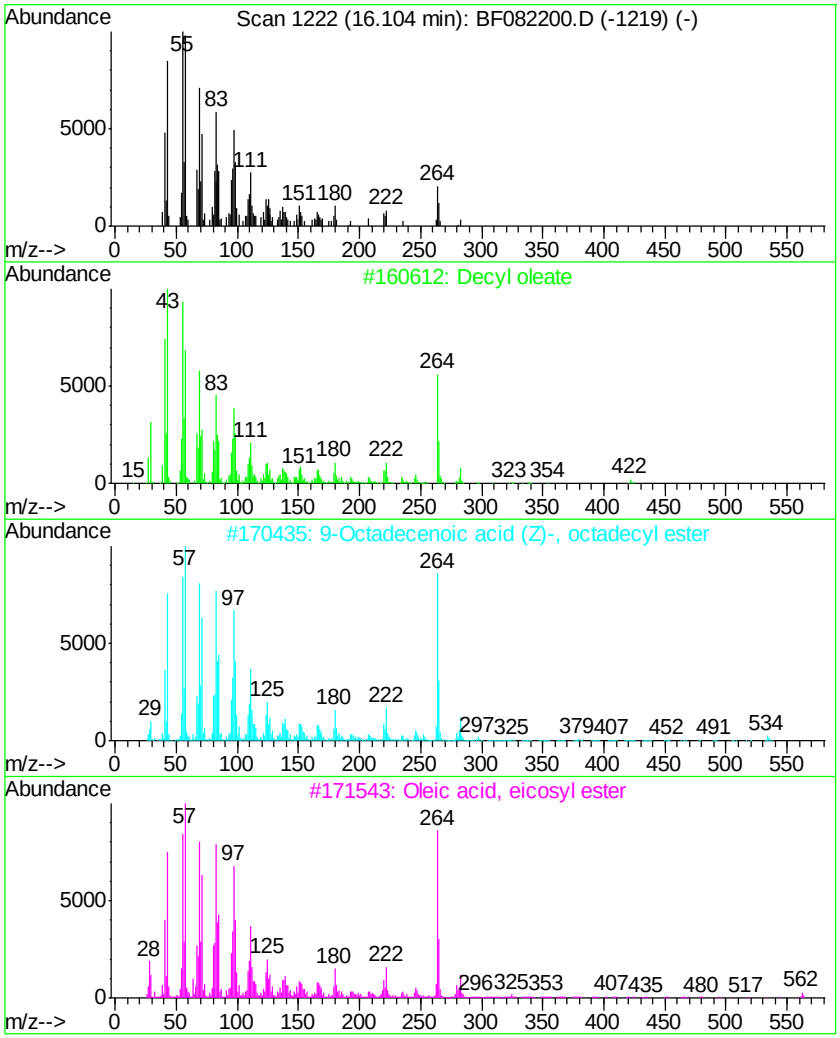
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

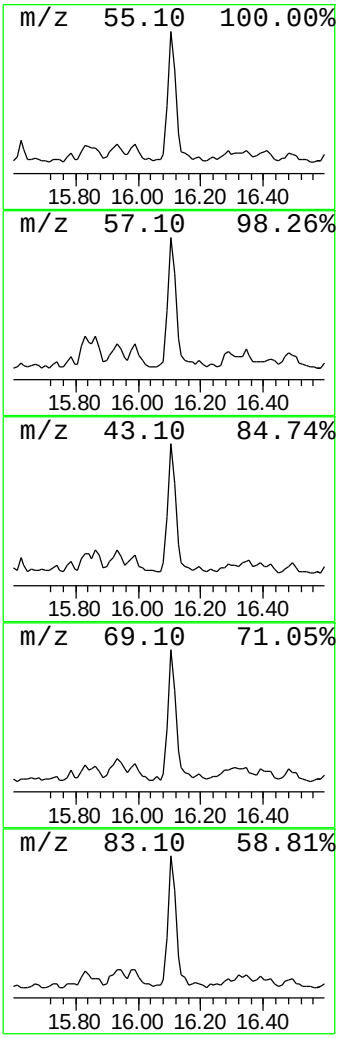
****

Peak Number 12 Decyl oleate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	9.21 ng	278136	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decyl oleate	422	C28H54O2	003687-46-5	91
2	9-Octadecenoic acid (Z)-, octade...	535	C36H70O2	017673-49-3	91
3	Oleic acid, eicosyl ester	563	C38H74O2	022393-88-0	91
4	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	87
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	76





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082200.D
Acq On : 11 Oct 2015 3:11
Operator : UM/IZ
Sample : G3959-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PO-002

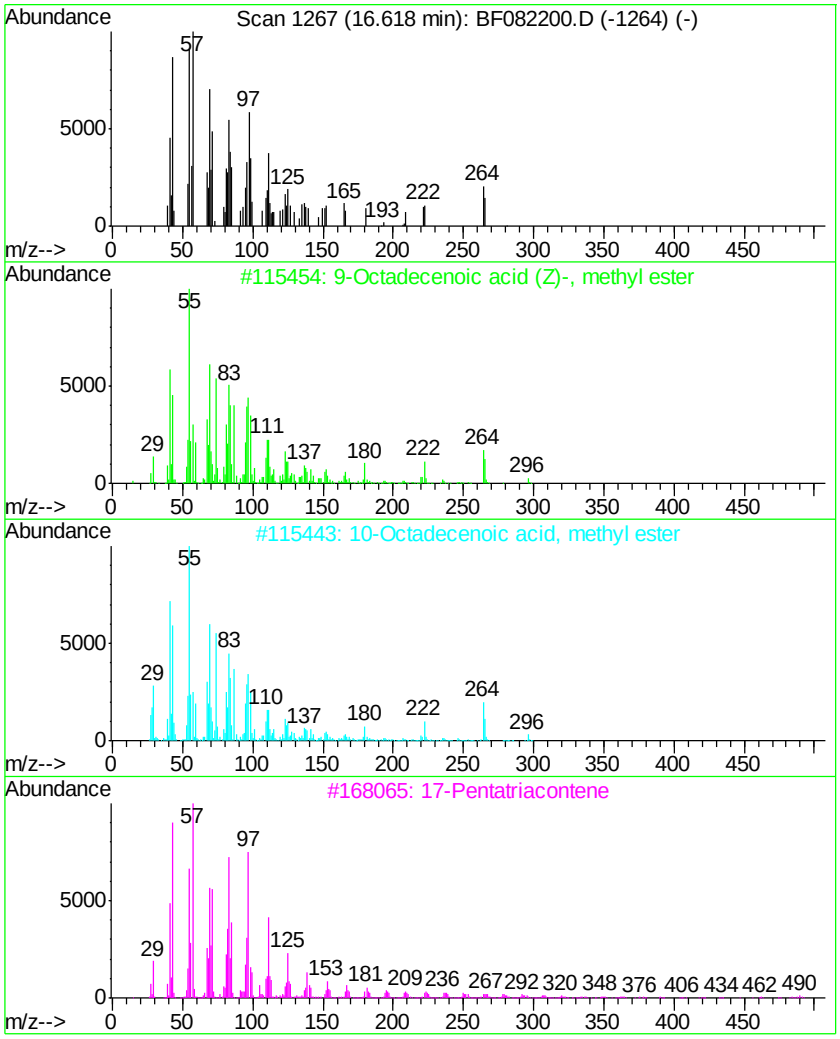
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

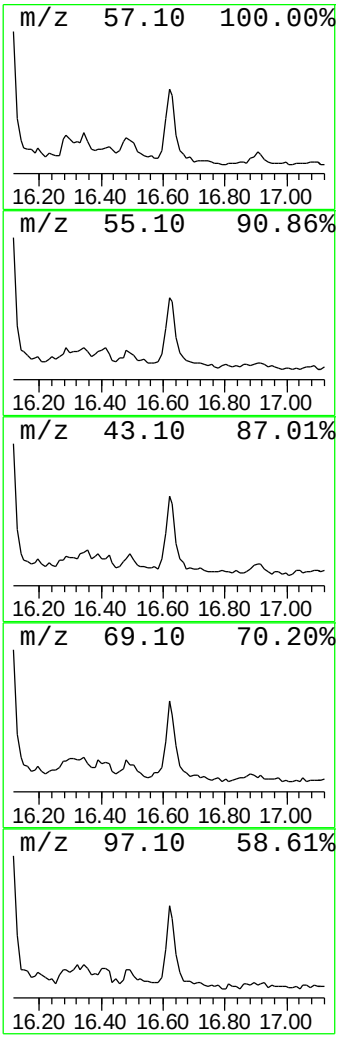
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.62	4.20 ng	126954	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	76
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	68
3	17-Pentatriacontene	491	C35H70	006971-40-0	60
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	55
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	55





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101015\
Data File : BF082200.D
Acq On : 11 Oct 2015 3:11
Operator : UM/IZ
Sample : G3959-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PO-002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	15.1	ng	396547	1	6.83	526723	20.0
unknown6.61	6.61	83.1	ng	2187680	1	6.83	526723	20.0
Benzenesulfonamid...	10.73	4.3	ng	173518	4	11.36	809389	20.0
n-Hexadecanoic acid	11.90	2.8	ng	112149	4	11.36	809389	20.0
Bromacil	11.97	8.7	ng	350897	4	11.36	809389	20.0
unknown13.56	13.56	2.2	ng	80209	5	14.00	724399	20.0
Trichloroacetic a...	13.85	3.7	ng	133738	5	14.00	724399	20.0
unknown14.42	14.42	2.2	ng	81061	5	14.00	724399	20.0
Decyl oleate	16.10	9.2	ng	278136	6	15.44	603841	20.0
9-Octadecenoic ac...	16.62	4.2	ng	126954	6	15.44	603841	20.0