LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

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-BF122415.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	4.967	251	252	261	rBB	60308	89390	5.00%	0.749%
2	5.413	290	291	301	rBV	510220	576945	32.29%	4.834%
3	6.453	380	382	390	rBB	384127	345027	19.31%	2.891%
4	6.567	390	392	395	rBV	938326	1057426	59.18%	8.860%
5	6.796	410	412	415	rBV	346284	289444	16.20%	2.425%
6	6.956	423	426	428	rBV	1221714	1165894	65.25%	9.769%
7	7.367	459	462	464	rBV	899078	933176	52.22%	7.819%
8	7.641	482	486	490	rBV3	11599	33392	1.87%	0.280%
9	8.019	513	519	522	rBV	32718	57210	3.20%	0.479%
10	8.087	522	525	527	rBV	294776	382005	21.38%	3.201%
11	8.304	542	544	547	rVB3	12260	27196	1.52%	0.228%
12	8.487	557	560	562	rBV	34466	48787	2.73%	0.409%
13	8.567	564	567	570	rVB5	14218	26843	1.50%	0.225%
14	8.613	570	571	574	rBV2	16563	23870	1.34%	0.200%
15	8.750	580	583	584	rBV2	9983	18641	1.04%	0.156%
16	8.796	584	587	588	rVV2	13623	30626	1.71%	0.257%
17	8.887	592	595	597	rVV2	22208	50091	2.80%	0.420%
18	8.956	599	601	604	rVB3	35388	56580	3.17%	0.474%
19	9.036	606	608	611	rVV3	23236	49648	2.78%	0.416%
20	9.093	611	613	616	rVV2	21107	39215	2.19%	0.329%
21	9.162	616	619	621	rVV	1913595	1786866	100.00%	14.972%
22	9.276	625	629	632	rBV3	18399	49509	2.77%	0.415%
23	9.344	633	635	637	rVB2	28388	32199	1.80%	0.270%
24	9.379	637	638	640	rVB	21082	19940	1.12%	0.167%
25	9.425	640	642	645	rBV	29500	41931	2.35%	0.351%
26	9.482	645	647	650	rBV3	37249	73938	4.14%	0.620%
27	9.562	652	654	658	rVB	77231	126381	7.07%	1.059%
28	9.653	658	662	663	rBV2	23870	44368	2.48%	0.372%
29	9.779	670	673	675	rBV3	22468	46128	2.58%	0.386%
30	9.836	675	678	680	rVV	485992	465257	26.04%	3.898%
31	9.905	683	684	687	rVV2	24425	29788	1.67%	0.250%
32	9.996	690	692	696	rVB5	12974	25410	1.42%	0.213%
33	10.053	696	697	700	rBV2	13789	30533	1.71%	0.256%
34	10.110	700	702	703	rVV2	27917	36999	2.07%	0.310%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

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-BF122415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.190	707	709	713	rVV2	44893	87606	4.90%	0.734%
36	10.270	713	716	718	rVB4	32612	46761	2.62%	0.392%
37	10.396	726	727	729	rBV2	22528	33577	1.88%	0.281%
38	10.522	736	738	740	rBV2	17434	22982	1.29%	0.193%
39	10.625	745	747	750	rBV	1049760	1015297	56.82%	8.507%
40	10.739	755	757	762	rVB3	22782	51846	2.90%	0.434%
41	11.185	793	796	798	rVB4	21634	39402	2.21%	0.330%
42	11.322	805	808	810	rBV	393541	408247	22.85%	3.421%
43	11.390	811	814	819	rVB3	10043	21699	1.21%	0.182%
44	11.859	853	855	860	rVB3	28918	36298	2.03%	0.304%
45	12.899	943	946	949	rBV	1348175	1335786	74.76%	11.192%
46	13.493	995	998	1000	rVB	97766	91272	5.11%	0.765%
47	13.802	1022	1025	1030	rVB3	22406	49939	2.79%	0.418%
48	13.951	1036	1038	1041	rBV	232472	314295	17.59%	2.633%
49	15.379	1160	1163	1172	rVB	200665	269342	15.07%	2.257%

Sum of corrected areas: 11935002

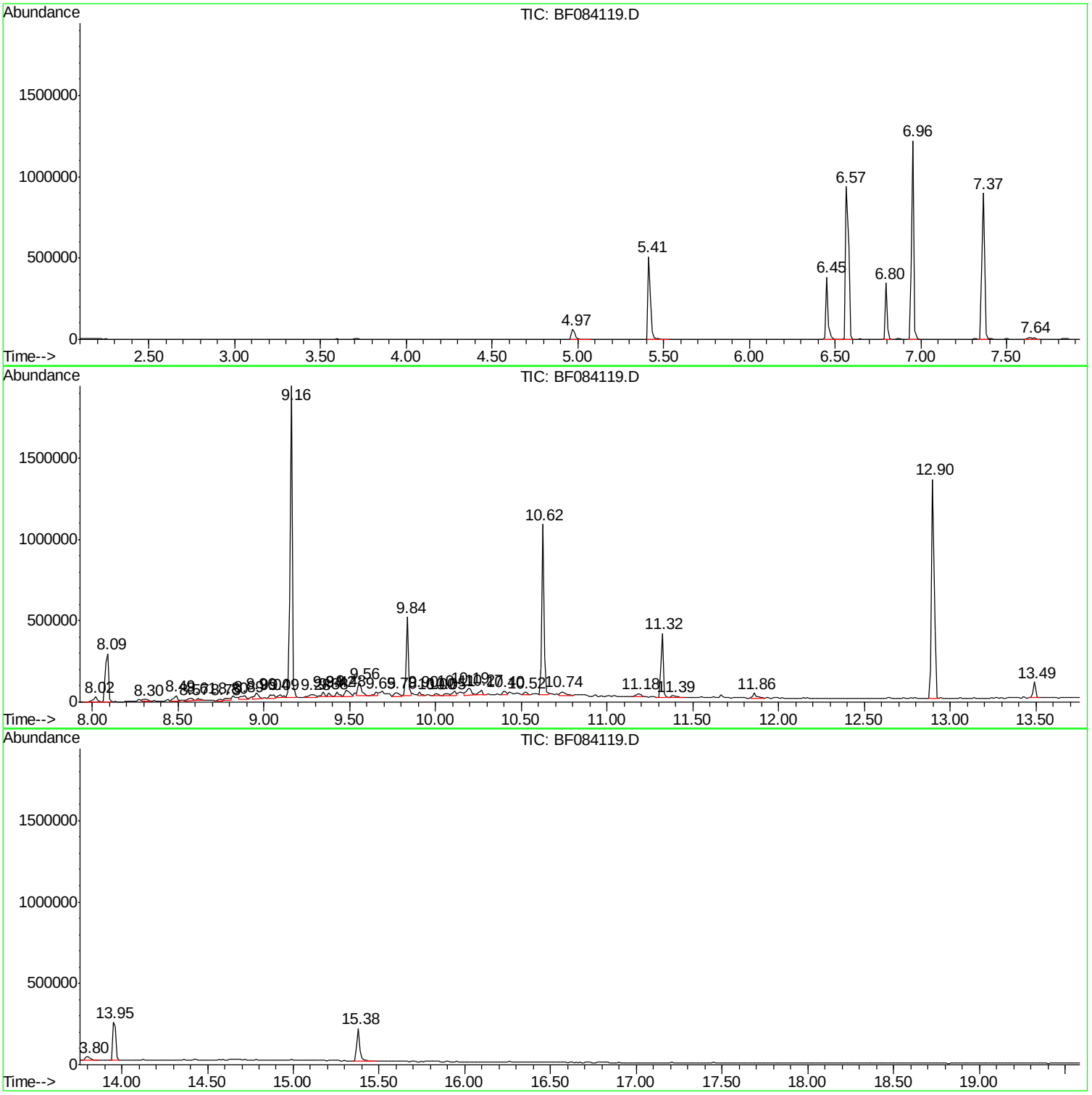
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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 : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

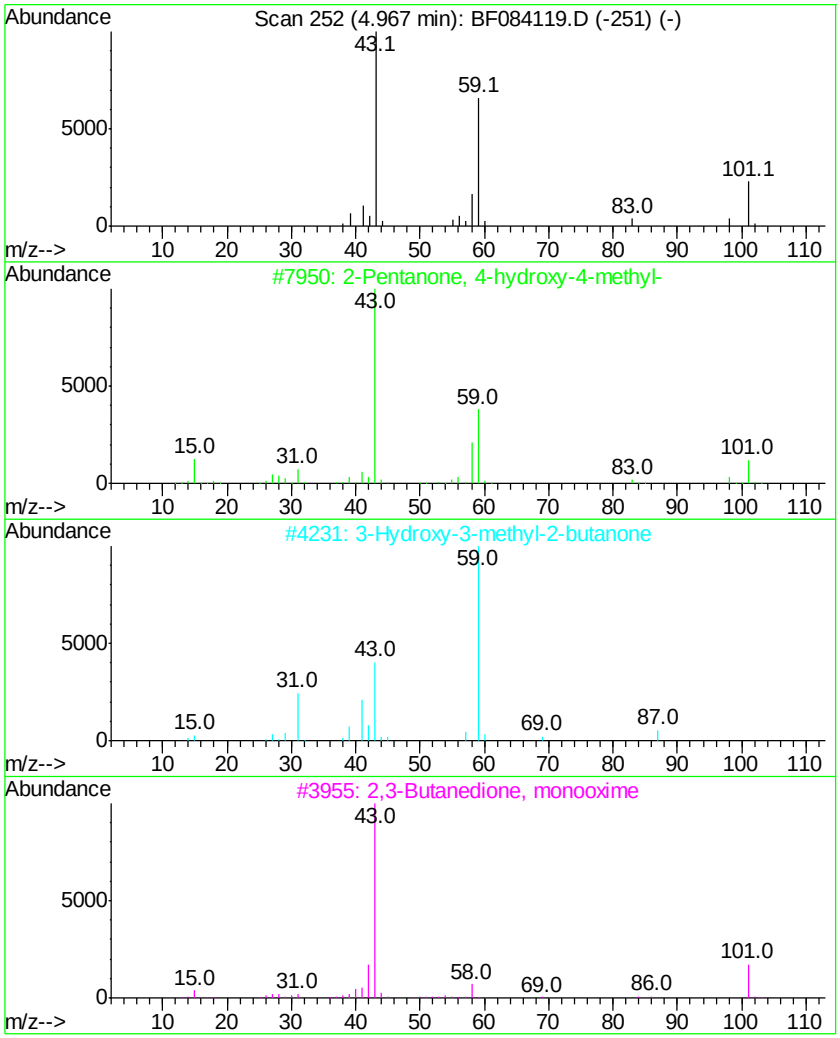
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

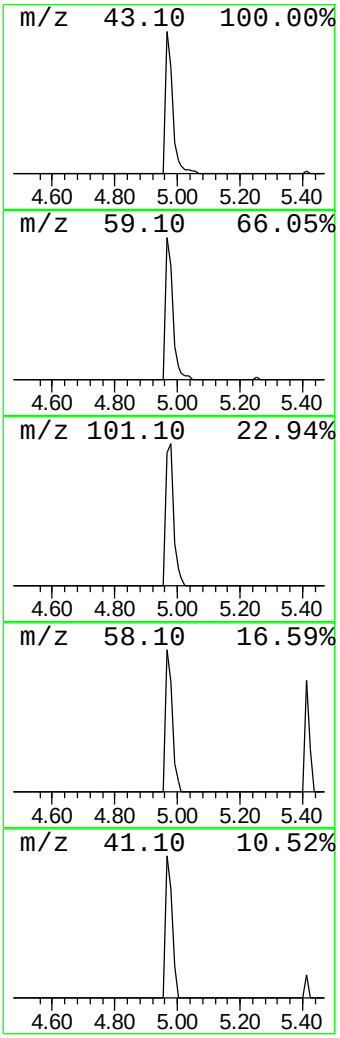
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	6.18 ng	89390	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

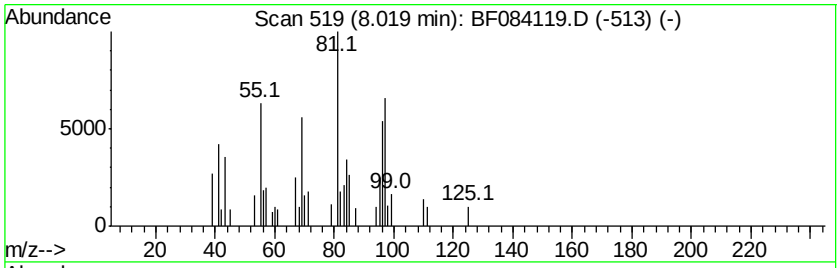
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

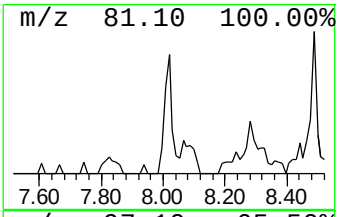
****

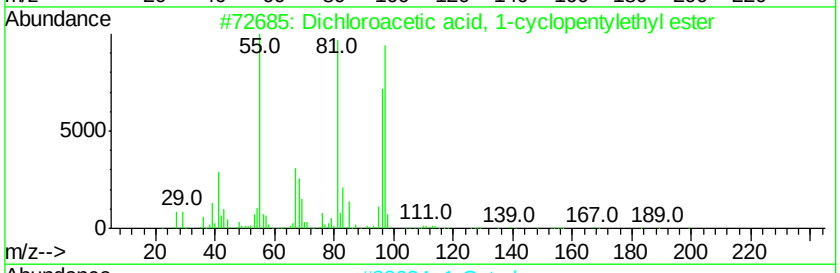
Peak Number 4 Dichloroacetic acid, 1-cycl... Concentration Rank 8

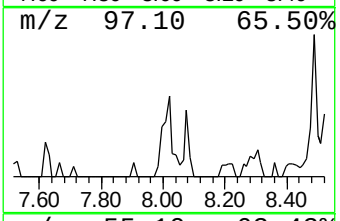
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.02	3.00 ng	57210	Naphthalene-d8	8.09

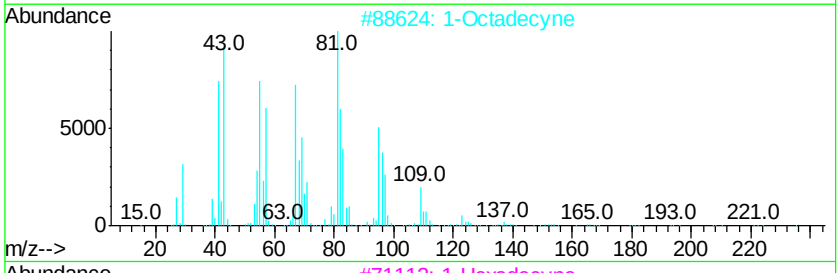
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, 1-cyclopent...	224	C9H14Cl2O2	1000282-56-3	50
2	1-Octadecyne	250	C18H34	000629-89-0	40
3	1-Hexadecyne	222	C16H30	000629-74-3	38
4	2-Butenenitrile, 2-amino-3-methyl-	96	C5H8N2	1000196-28-0	37
5	1-Pentadecyne	208	C15H28	000765-13-9	35

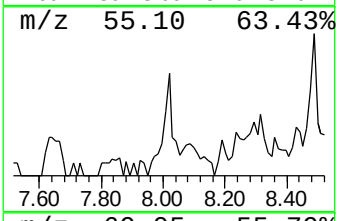


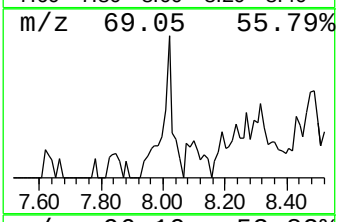


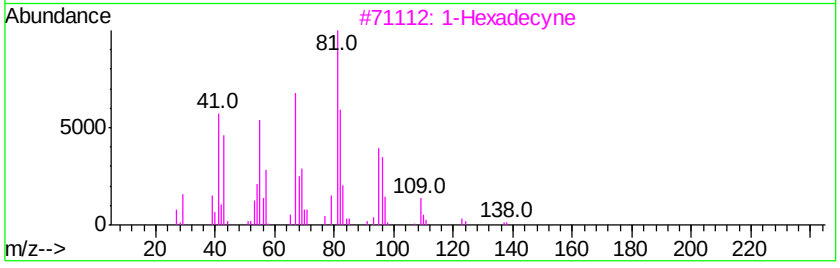


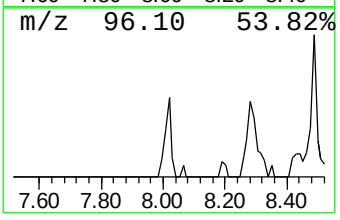












Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
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Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

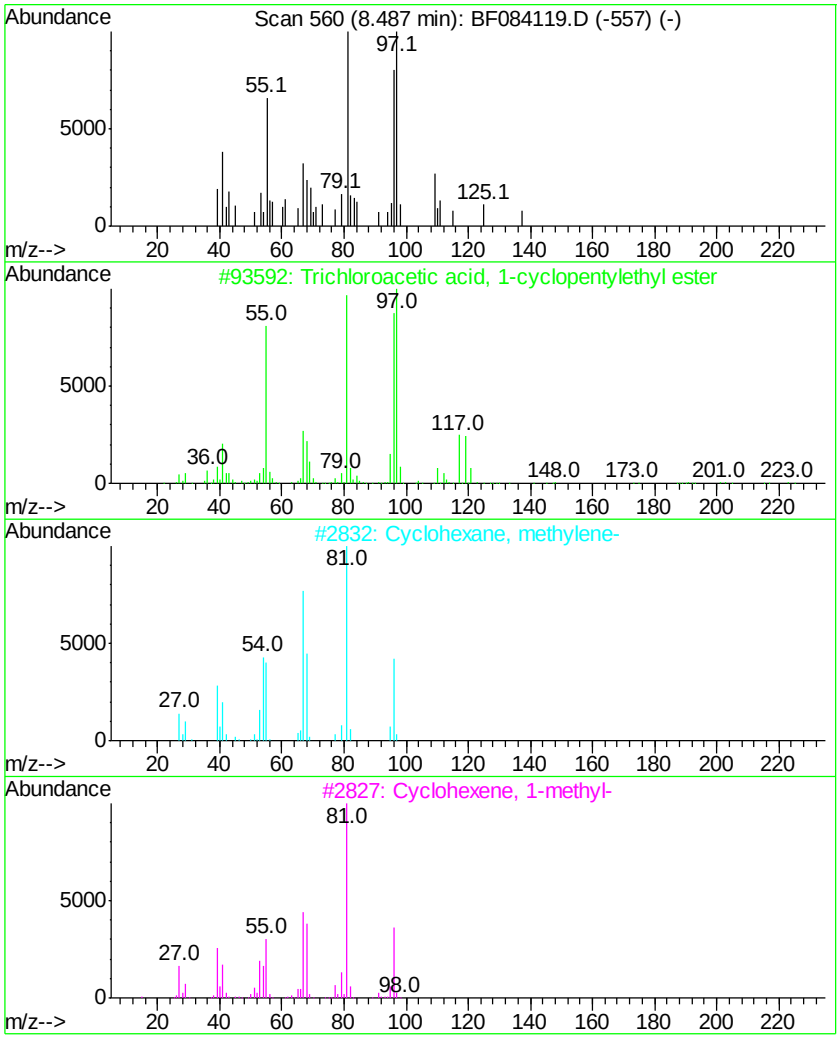
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

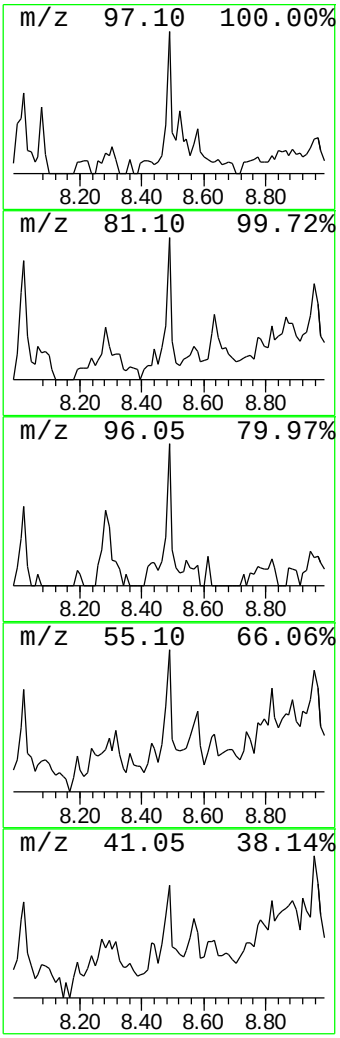
****

Peak Number 5 Trichloroacetic acid, 1-cyc... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.49	2.55 ng	48787	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, 1-cyclopen...	258	C9H13Cl3O2	1000282-57-1	80
2	Cyclohexane, methylene-	96	C7H12	001192-37-6	43
3	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	43
4	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	43
5	1-(2-Methylpropenyl)aziridine	97	C6H11N	080839-93-6	43





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Data File : BF084119.D
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Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

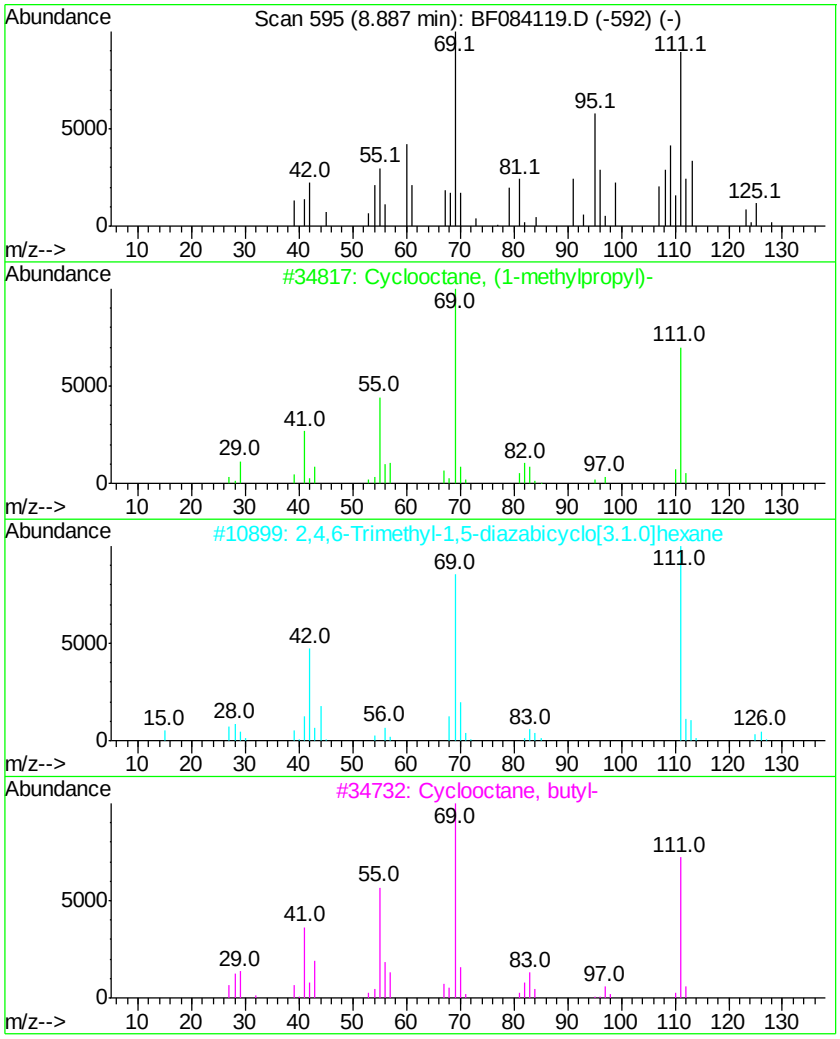
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

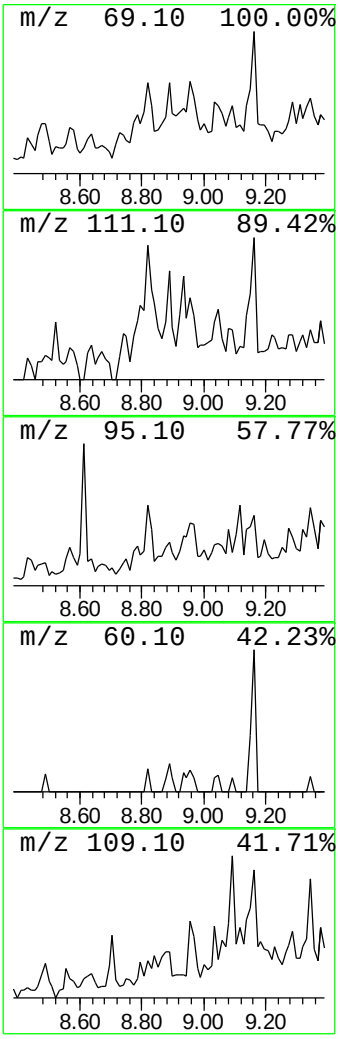
****

Peak Number 6 unknown8.89 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	2.62 ng	50091	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	35
2	2,4,6-Trimethyl-1,5-diazabicyclo...	126	C7H14N2	1000283-21-2	35
3	Cyclooctane, butyl-	168	C12H24	016538-93-5	27
4	Cyclohexane, 1-ethyl-1,3-dimethy...	140	C10H20	062238-29-3	25
5	Methoxyacetic acid, 2-ethylcyclo...	200	C11H20O3	1000282-69-7	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
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Acq On : 25 Dec 2015 10:14
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Sample : G4951-12
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ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

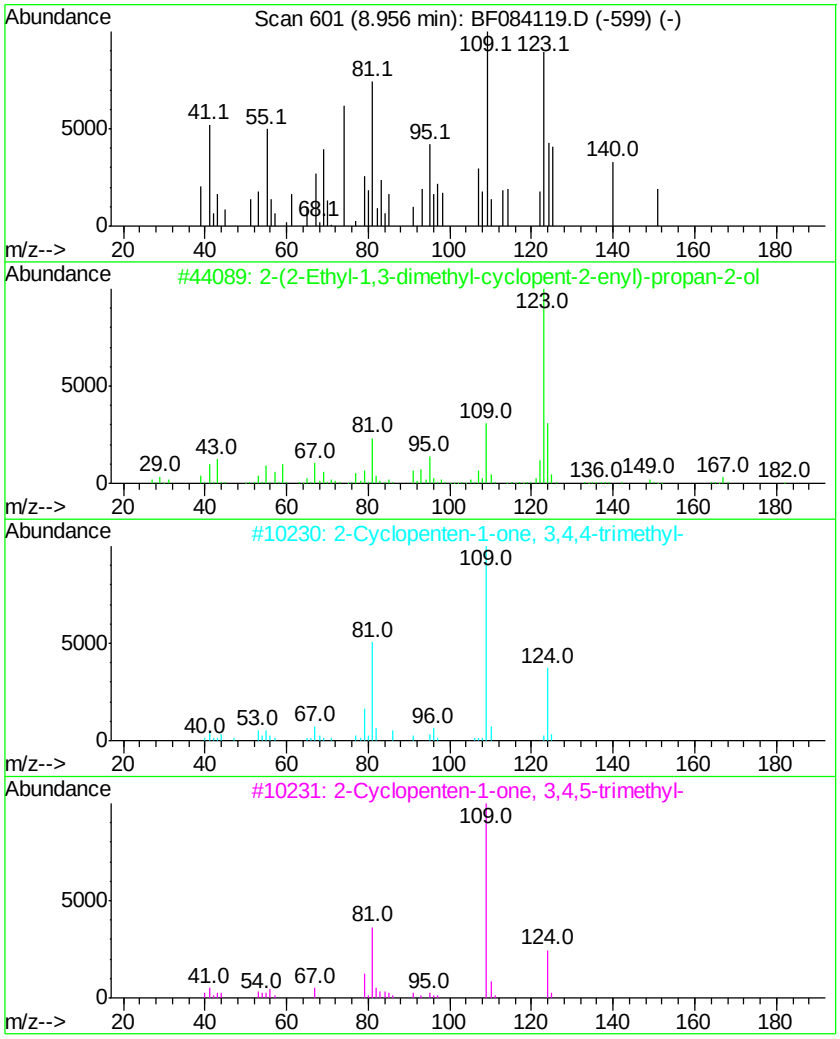
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

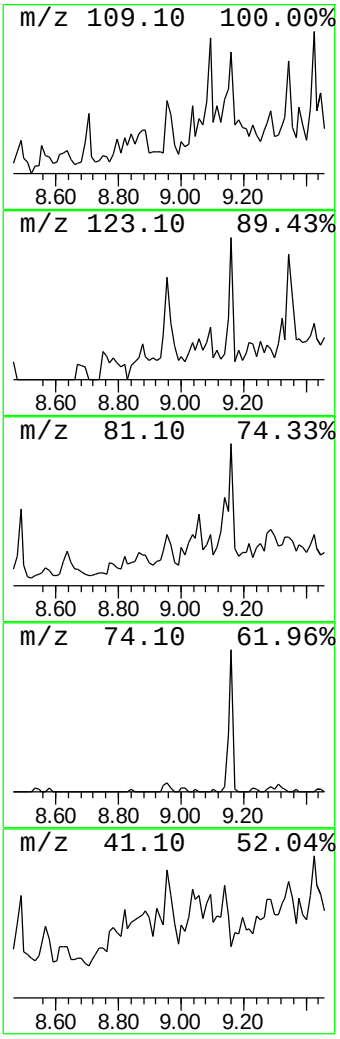
****

Peak Number 7 unknown8.96 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	2.96 ng	56580	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-Ethyl-1,3-dimethyl-cyclopen...	182	C12H22O	1000186-82-4	43
2	2-Cyclopenten-1-one, 3,4,4-trime...	124	C8H12O	030434-65-2	43
3	2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	41
4	Cyclopent-2-ene-1-one, 2,3,4-tri...	124	C8H12O	083321-16-8	38
5	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	38





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Data File : BF084119.D
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Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

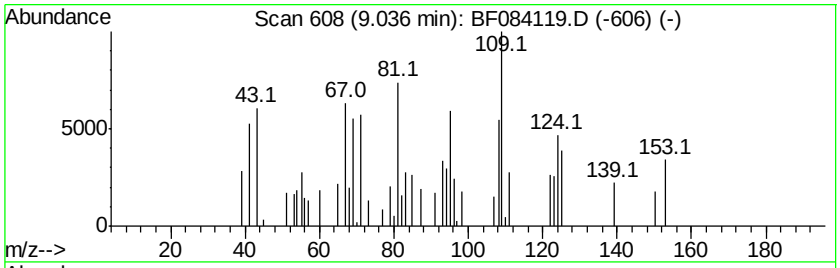
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

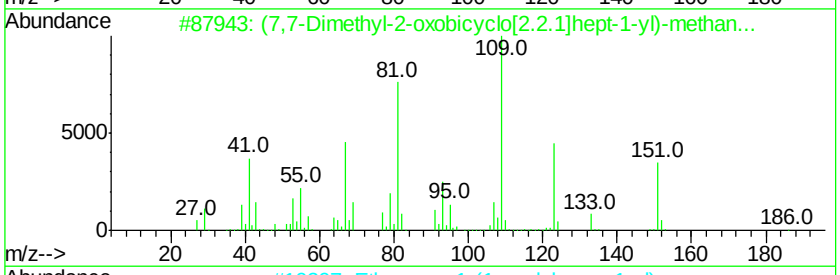
****

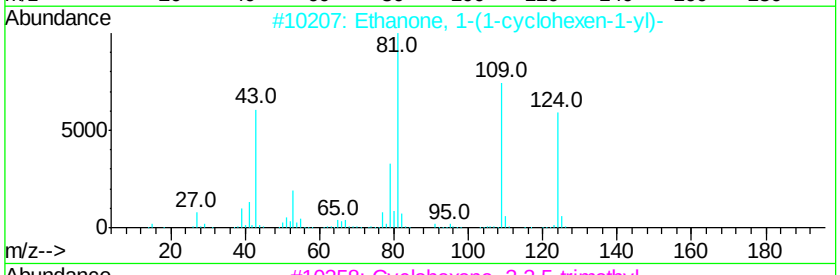
Peak Number 8 unknown9.04 Concentration Rank 13

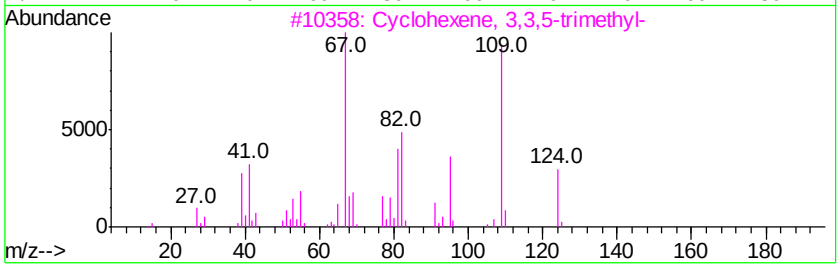
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	2.13 ng	49648	Acenaphthene-d10	9.84

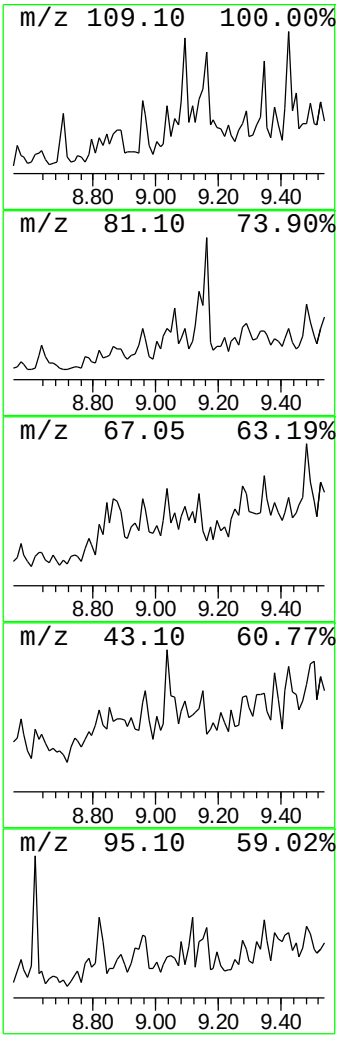
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	38
2	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	30
3	Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	30
4	Cyclohexane, (1-methylethylidene)-	124	C9H16	005749-72-4	25
5	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	18











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ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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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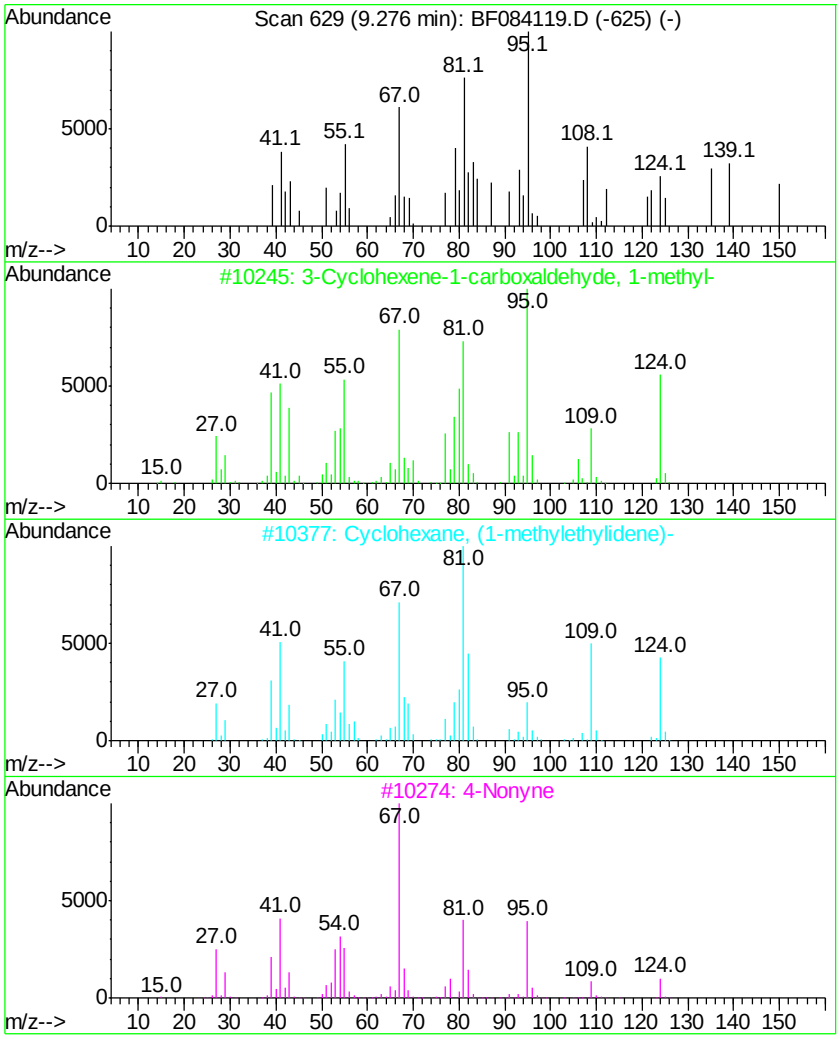
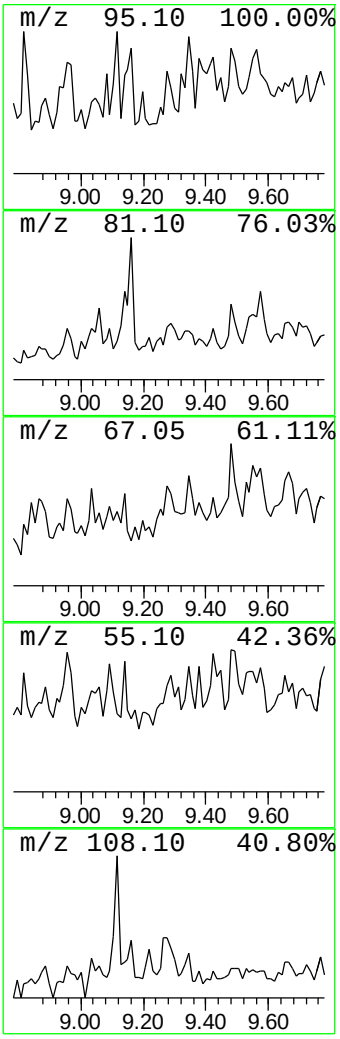
Peak Number 9 unknown9.28 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.28	2.13 ng	49509	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-carboxaldehyde, ...	124	C8H12O	000931-96-4	38
2	Cyclohexane, (1-methylethylidene)-	124	C9H16	005749-72-4	35
3	4-Nonyne	124	C9H16	020184-91-2	25
4	1,5-Cyclooctadiene, 1-t-butyl-	164	C12H20	1000152-18-6	22
5	1,4-Pentadiene, 3-propyl-	110	C8H14	000996-83-8	22





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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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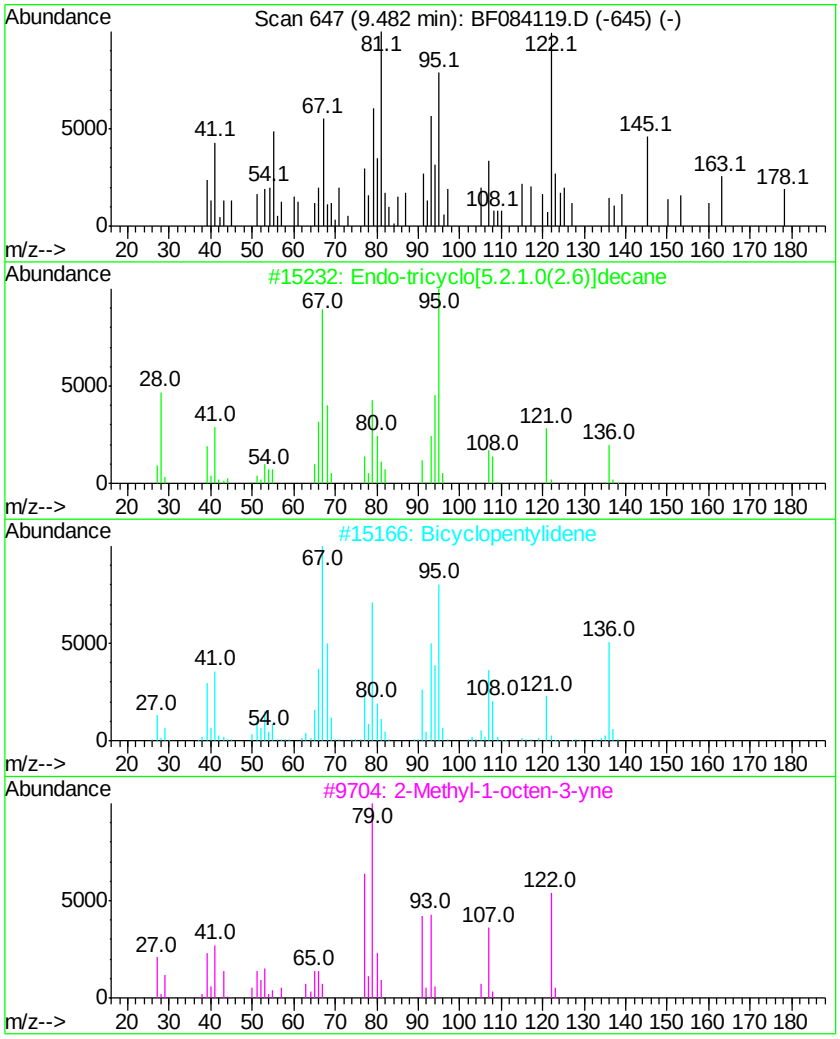
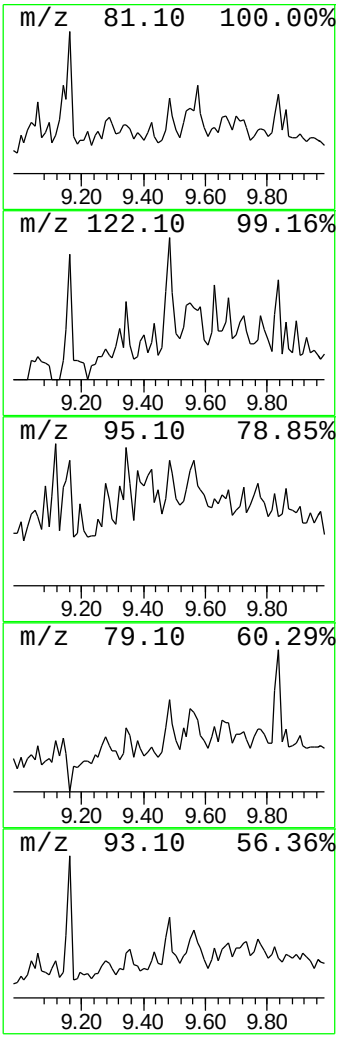
Peak Number 10 unknown9.48 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	3.18 ng	73938	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Endo-tricyclo[5.2.1.0(2.6)]decane	136	C10H16	1000215-28-8	30
2	Bicyclopentylidene	136	C10H16	016189-35-8	30
3	2-Methyl-1-octen-3-yne	122	C9H14	017603-76-8	25
4	3-Pyridinecarboxylic acid, 1,2-d...	139	C6H5NO3	000609-71-2	25
5	3-Methylene-2-norbornanone	122	C8H10O	005597-27-3	22





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Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
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TIC Library : C:\DATABASE\NIST02.L
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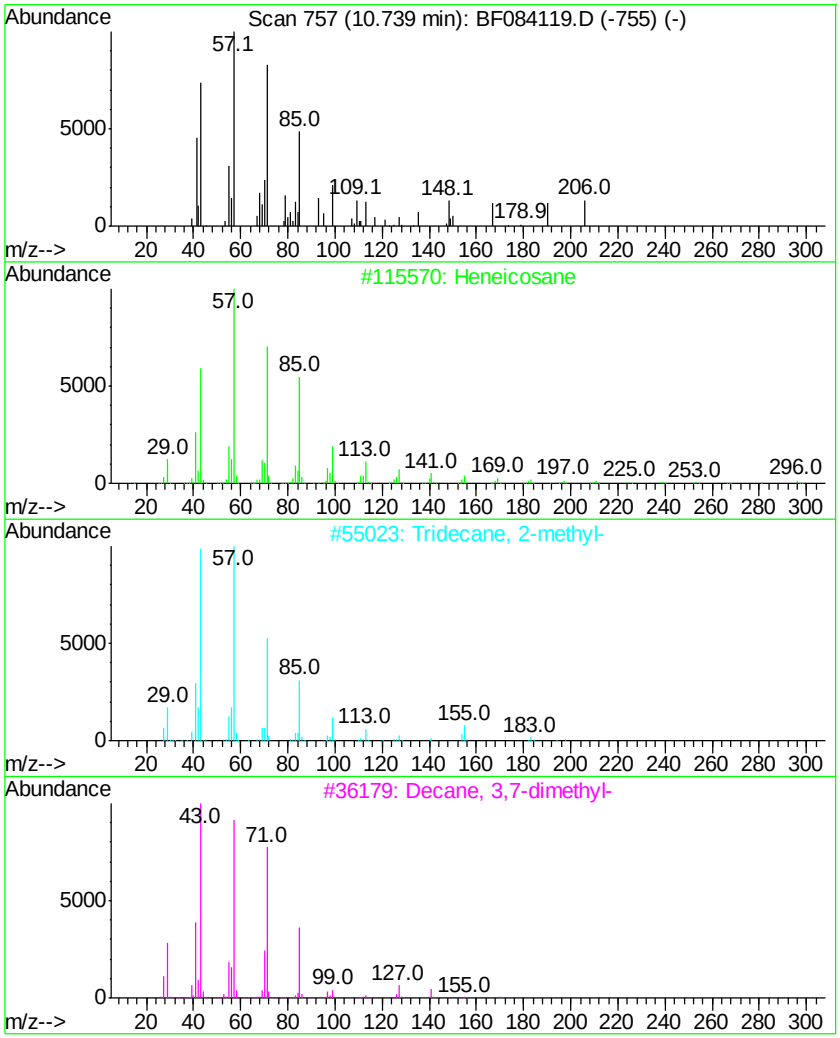
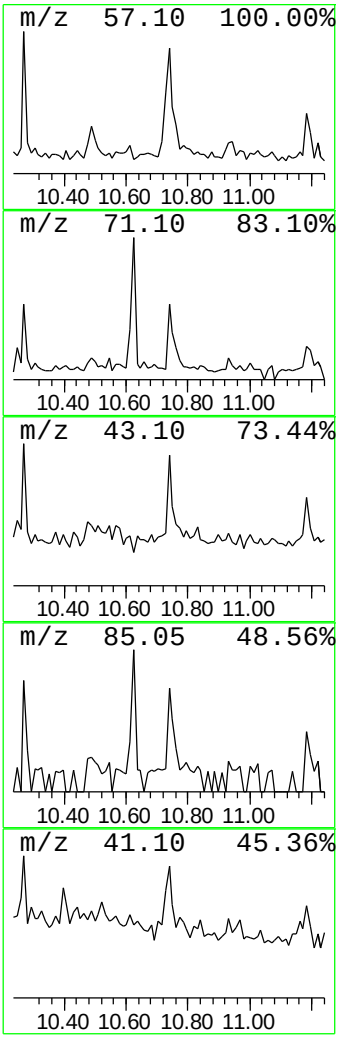
Peak Number 13 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	2.54 ng	51846	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	53
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	50
3	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	50
4	Tetradecane	198	C14H30	000629-59-4	50
5	Hexadecane	226	C16H34	000544-76-3	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
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Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
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TIC Library : C:\DATABASE\NIST02.L
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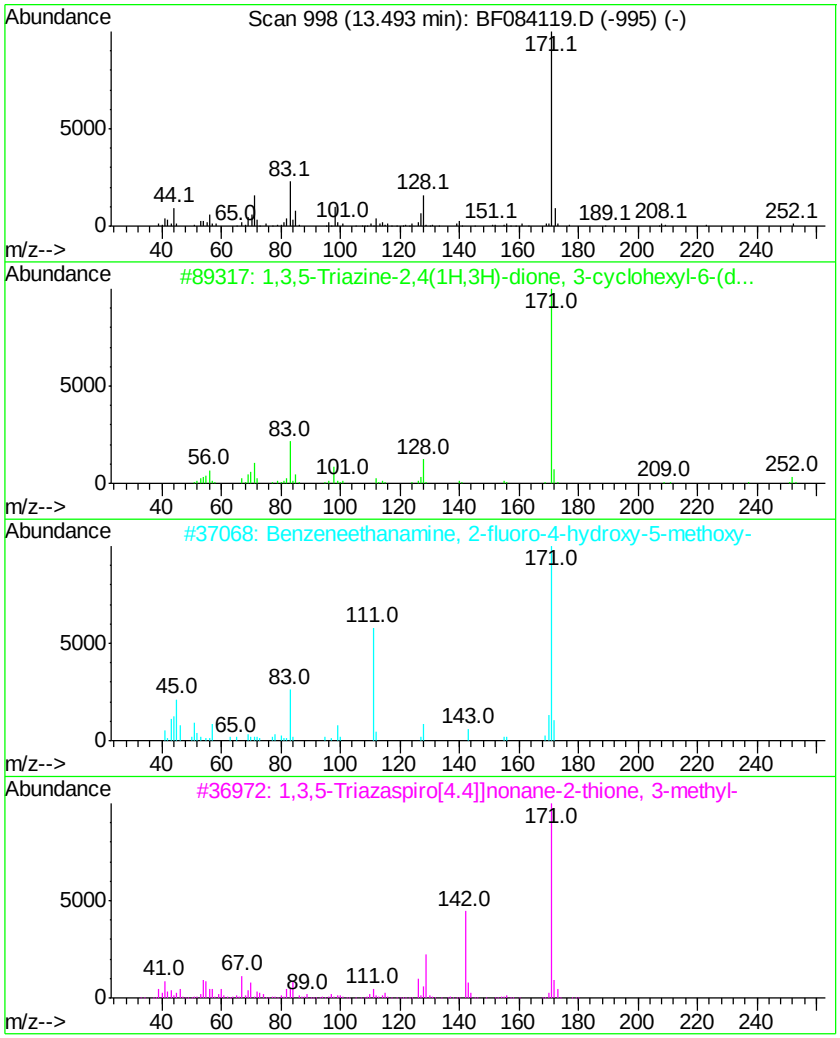
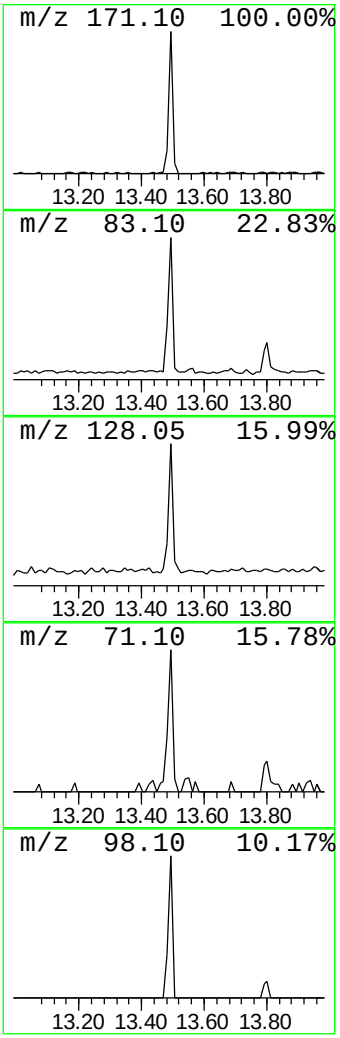
Peak Number 14 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	5.81 ng	91272	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	94
2	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FNO2	1000116-43-3	50
3	1,3,5-Triazaspiro[4.4]nonane-2-...	171	C7H13N3S	1000277-58-6	40
4	Benzeneethanamine, 2-fluoro-.bet...	201	C9H12FNO3	099387-72-1	39
5	2,7-dithiatricyclo[4.3.1.0(3,8)]...	250	C8H11BrS2	1000197-96-2	37





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084119.D
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Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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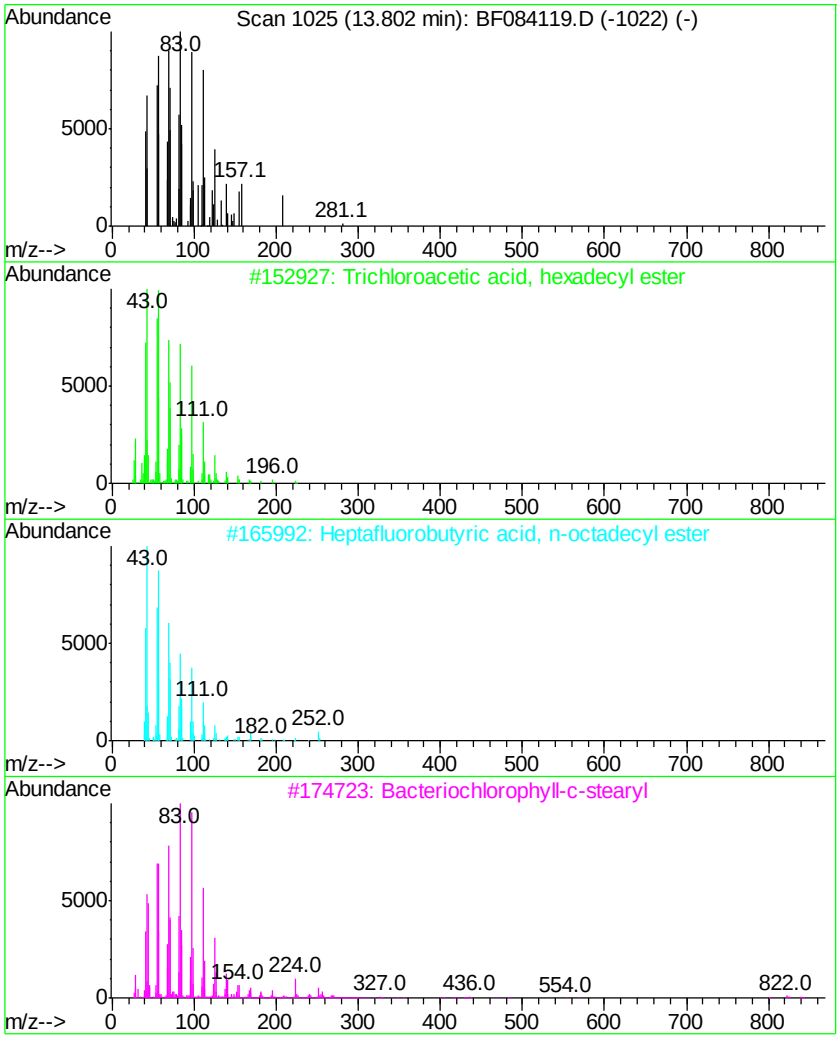
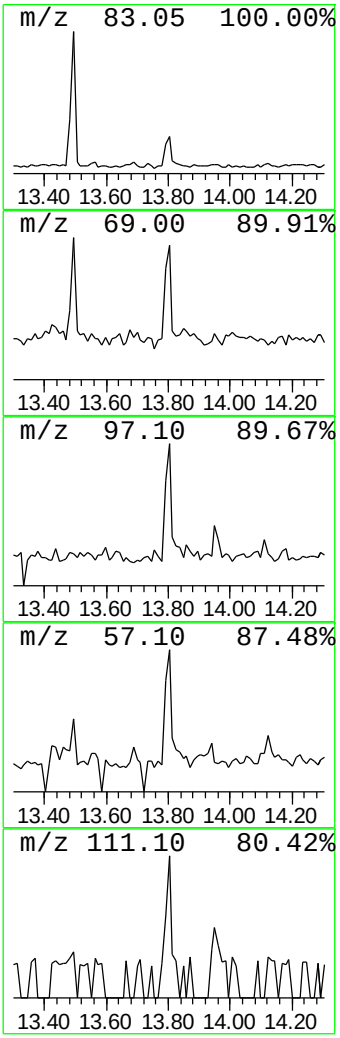
Peak Number 15 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.18 ng	49939	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	74
3	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	72
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	68
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084119.D
Acq On : 25 Dec 2015 10:14
Operator : UM/SJ
Sample : G4951-12
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-6-122315

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122415.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
2-Pentanone, 4-hy...	4.97	6.2	ng	89390	1	6.80	289444	20.0
Dichloroacetic ac...	8.02	3.0	ng	57210	2	8.09	382005	20.0
Trichloroacetic a...	8.49	2.5	ng	48787	2	8.09	382005	20.0
unknown8.89	8.89	2.6	ng	50091	2	8.09	382005	20.0
unknown8.96	8.96	3.0	ng	56580	2	8.09	382005	20.0
unknown9.04	9.04	2.1	ng	49648	3	9.84	465257	20.0
unknown9.28	9.28	2.1	ng	49509	3	9.84	465257	20.0
unknown9.48	9.48	3.2	ng	73938	3	9.84	465257	20.0
Heneicosane	10.74	2.5	ng	51846	4	11.32	408247	20.0
1,3,5-Triazine-2,...	13.49	5.8	ng	91272	5	13.96	314295	20.0
Trichloroacetic a...	13.80	3.2	ng	49939	5	13.96	314295	20.0