LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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	250	252	261	rVB	95364	112650	6.32%	0.938%
2	5.413	290	291	303	rBB	516856	561777	31.53%	4.680%
3	6.453	380	382	390	rVB	383380	346602	19.45%	2.887%
4	6.567	390	392	395	rBV	880709	1016435	57.04%	8.467%
5	6.796	410	412	415	rBV	340613	286754	16.09%	2.389%
6	6.956	423	426	428	rBV	1151918	1107960	62.18%	9.229%
7	7.367	459	462	464	rBV	845891	893233	50.13%	7.441%
8	7.493	470	473	477	rVB2	17958	25858	1.45%	0.215%
9	7.825	499	502	506	rBV3	11994	26969	1.51%	0.225%
10	8.019	514	519	523	rBV4	33758	58835	3.30%	0.490%
11	8.088	523	525	527	rBV	338943	396856	22.27%	3.306%
12	8.225	532	537	539	rBV3	11020	32883	1.85%	0.274%
13	8.328	544	546	547	rVB	17679	19781	1.11%	0.165%
14	8.465	557	558	561	rBV2	14765	28983	1.63%	0.241%
15	8.556	565	566	569	rBV2	13207	23250	1.30%	0.194%
16	8.613	569	571	572	rBV	25772	20235	1.14%	0.169%
17	8.750	580	583	584	rVB2	13200	23105	1.30%	0.192%
18	8.796	584	587	588	rBV2	14571	33448	1.88%	0.279%
19	8.819	588	589	592	rVV3	21814	32433	1.82%	0.270%
20	8.888	592	595	596	rVV3	13767	25516	1.43%	0.213%
21	8.956	599	601	604	rVB3	22637	40178	2.25%	0.335%
22	9.059	606	610	611	rVV3	21005	45855	2.57%	0.382%
23	9.093	611	613	614	rVV	17965	30429	1.71%	0.253%
24	9.162	616	619	621	rVV	1936528	1781971	100.00%	14.844%
25	9.288	627	630	631	rBV2	18480	30486	1.71%	0.254%
26	9.345	633	635	637	rVB2	43504	48291	2.71%	0.402%
27	9.425	640	642	645	rBV3	24500	41623	2.34%	0.347%
28	9.482	645	647	650	rBV3	31604	65173	3.66%	0.543%
29	9.562	650	654	658	rVB3	30833	85160	4.78%	0.709%
30	9.653	658	662	663	rBV4	23257	48900	2.74%	0.407%
31	9.768	670	672	675	rBV4	20906	46194	2.59%	0.385%
32	9.836	675	678	680	rBV	495736	468351	26.28%	3.901%
33	9.996	691	692	696	rBV4	13109	29956	1.68%	0.250%
34	10.111	700	702	703	rVV2	27274	37330	2.09%	0.311%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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	10.145	703	705	707	rVV2	28660	47725	2.68%	0.398%
36	10.191	707	709	713	rVV4	41263	85362	4.79%	0.711%
37	10.271	713	716	718	rVB3	28290	42764	2.40%	0.356%
38	10.362	722	724	725	rBV	22110	25918	1.45%	0.216%
39	10.408	725	728	729	rBV3	17678	27001	1.52%	0.225%
40	10.533	736	739	740	rBV3	13161	18960	1.06%	0.158%
41	10.591	740	744	745	rBV3	19604	34870	1.96%	0.290%
42	10.625	745	747	750	rBV	1015788	1005689	56.44%	8.378%
43	10.739	755	757	759	rVV2	24133	35197	1.98%	0.293%
44	10.842	762	766	771	rVB7	14597	54931	3.08%	0.458%
45	11.185	793	796	798	rBV2	33893	52807	2.96%	0.440%
46	11.322	806	808	810	rBV	425947	408901	22.95%	3.406%
47	11.402	810	815	819	rVB7	11146	36413	2.04%	0.303%
48	11.665	836	838	842	rVB	31612	34774	1.95%	0.290%
49	11.859	853	855	859	rVB3	39179	53177	2.98%	0.443%
50	12.637	921	923	928	rBV6	10931	20914	1.17%	0.174%
51	12.728	929	931	933	rBV	24092	21370	1.20%	0.178%
52	12.899	944	946	949	rBV	1332065	1395131	78.29%	11.622%
53	13.494	995	998	1000	rVB	85177	81940	4.60%	0.683%
54	13.802	1023	1025	1029	rBV3	26521	51345	2.88%	0.428%
55	13.951	1036	1038	1041	rBV	250453	329141	18.47%	2.742%
56	15.380	1161	1163	1171	rVB	200190	266841	14.97%	2.223%

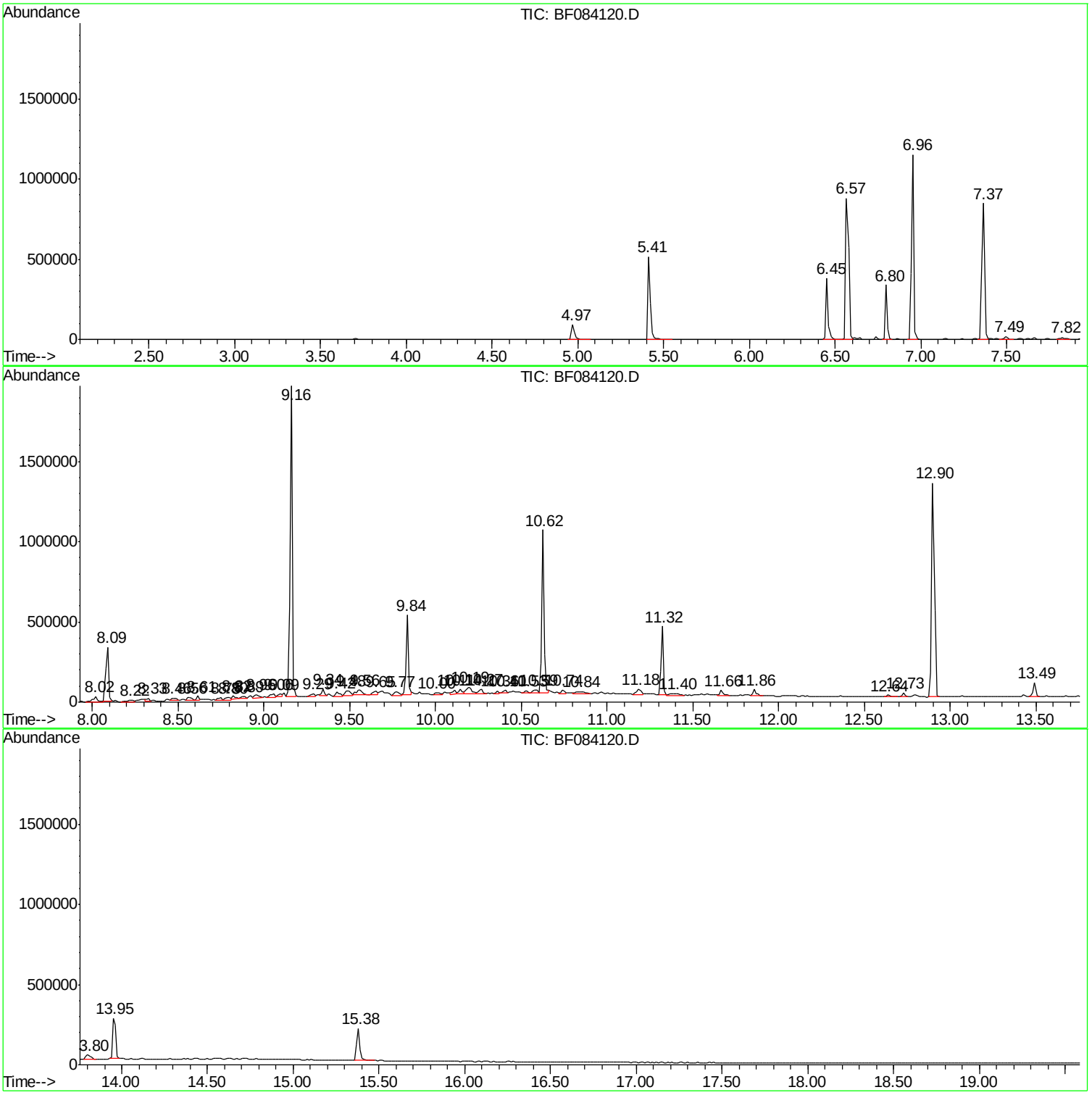
Sum of corrected areas: 12004631

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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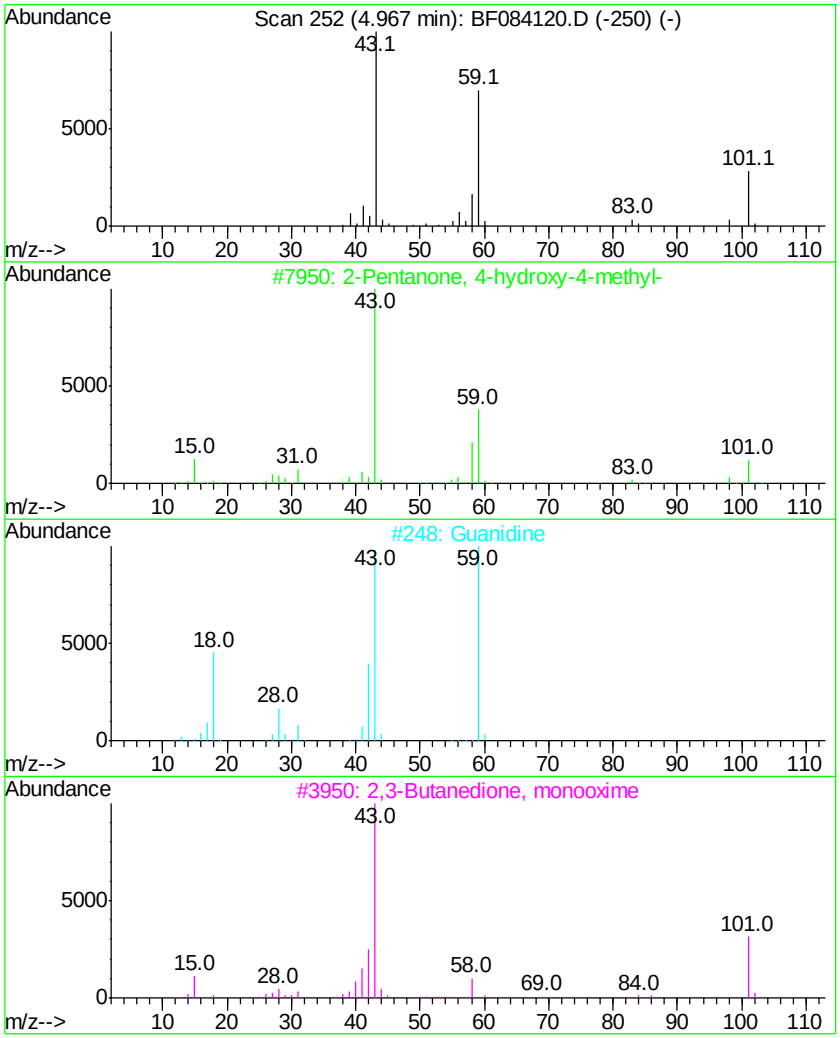
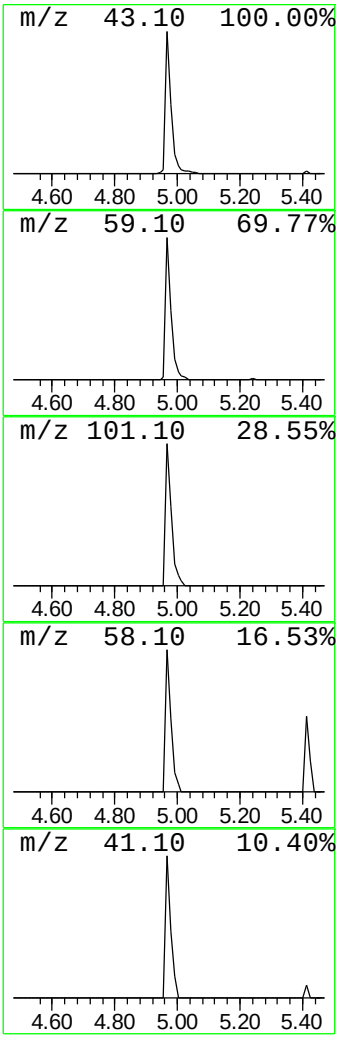
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	7.86 ng	112650	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	50
2	Guanidine	59	CH5N3	000113-00-8	43
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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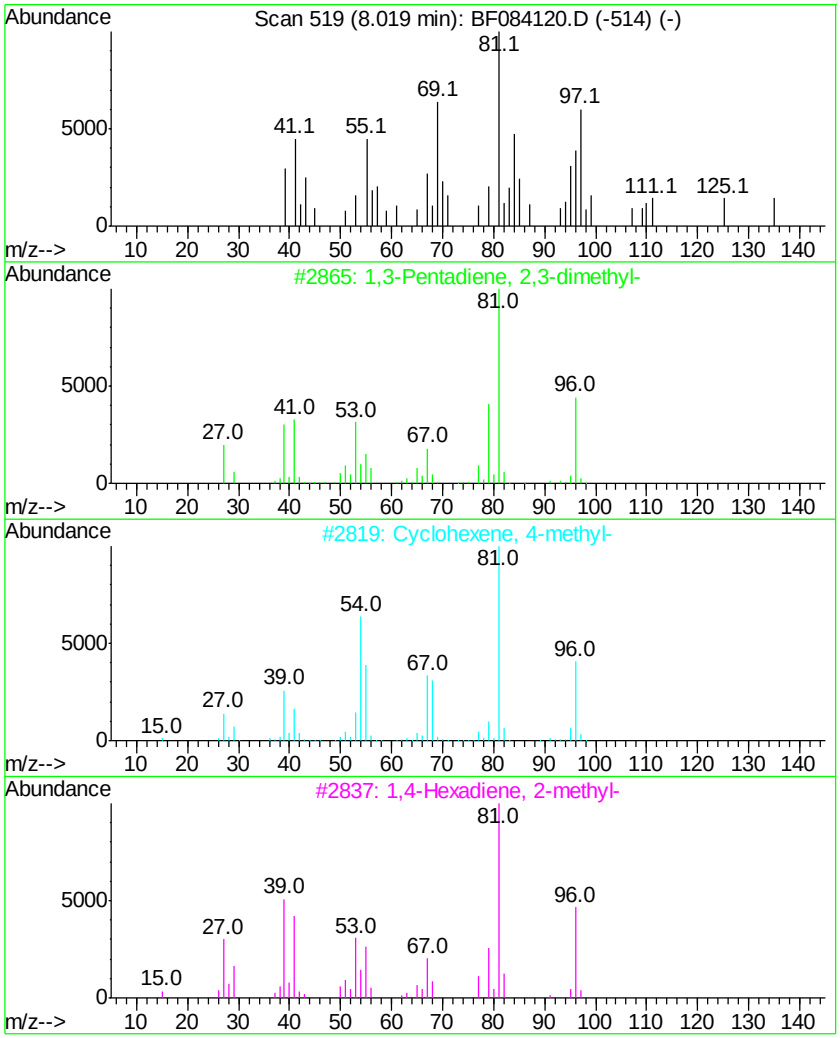
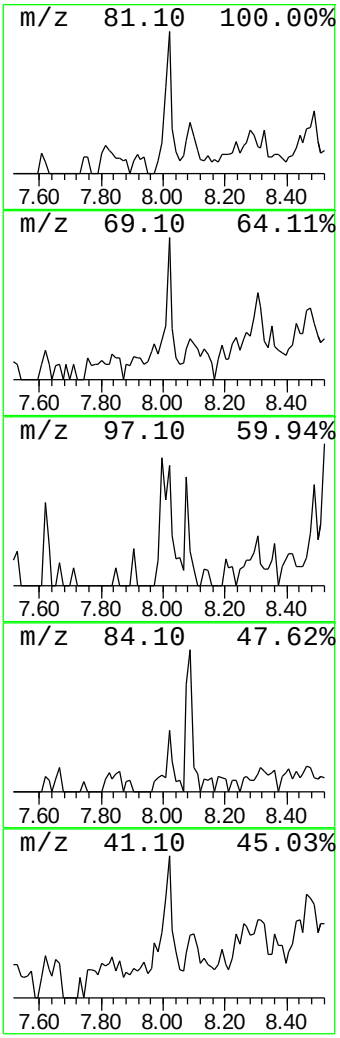
Peak Number 4 unknown8.02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.02	2.97 ng	58835	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Pentadiene, 2,3-dimethyl-	96	C7H12	001113-56-0	35
2	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	35
3	1,4-Hexadiene, 2-methyl-	96	C7H12	001119-14-8	35
4	2-Hexyne, 4-methyl-	96	C7H12	020198-49-6	35
5	1,4-Hexadiene, 5-methyl-	96	C7H12	000763-88-2	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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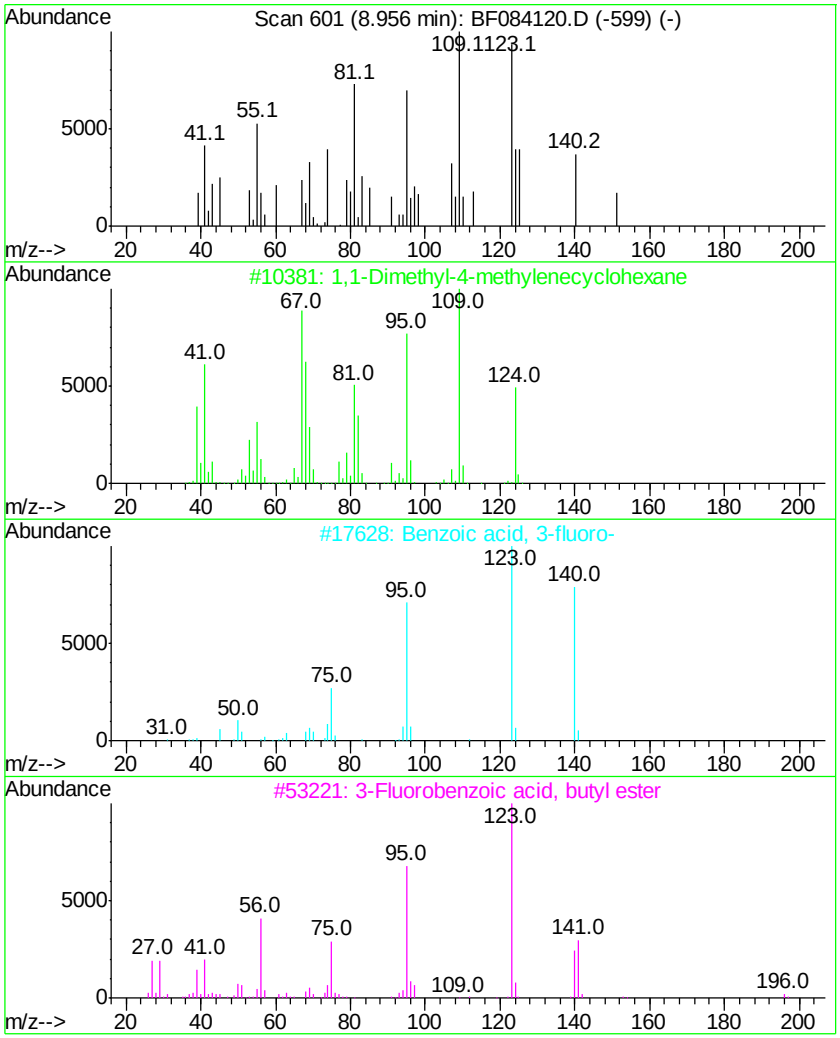
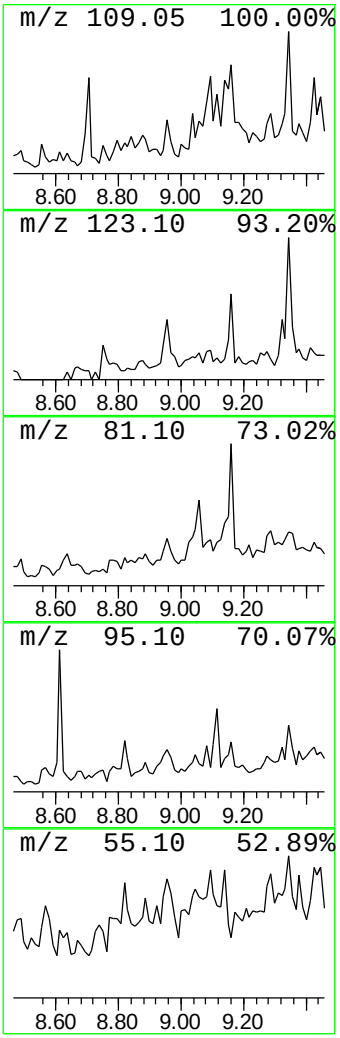
Peak Number 5 unknown8.96 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	2.02 ng	40178	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	30
2	Benzoic acid, 3-fluoro-	140	C7H5FO2	000455-38-9	25
3	3-Fluorobenzoic acid, butyl ester	196	C11H13FO2	077206-91-8	22
4	Hexahydroindole	123	C8H13N	018159-32-5	18
5	Ethanone, 1-(2-methyl-1-cyclopen...	124	C8H12O	003168-90-9	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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

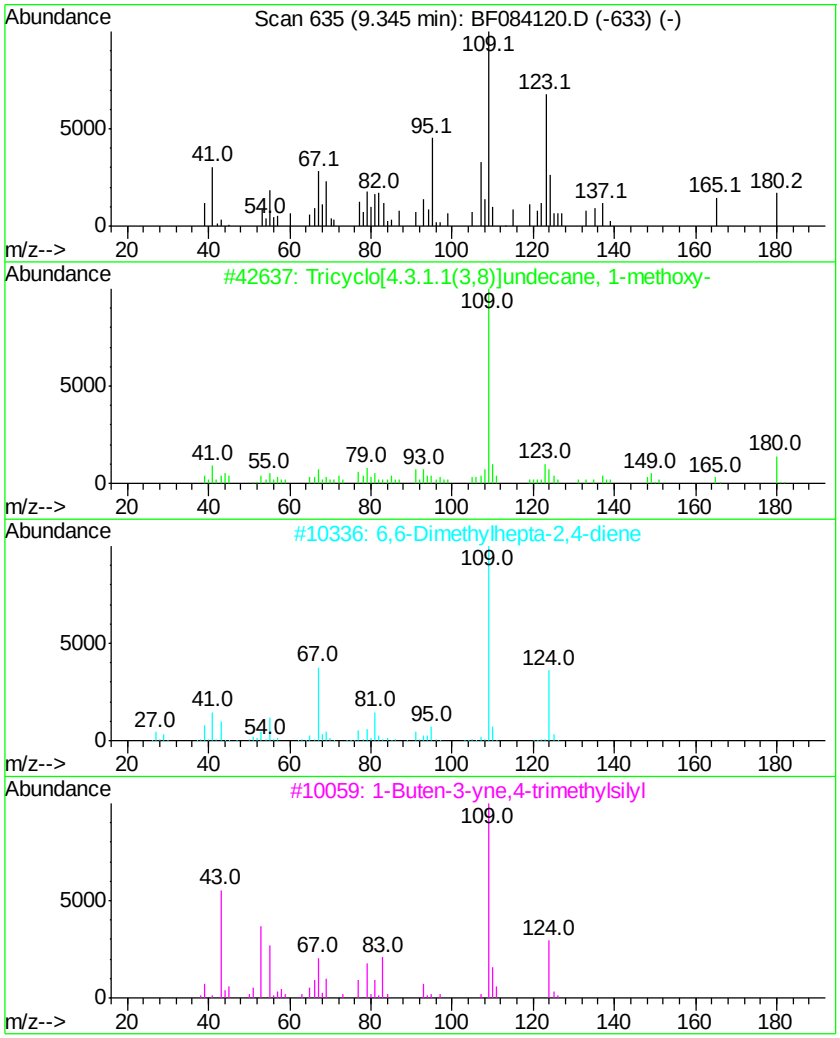
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

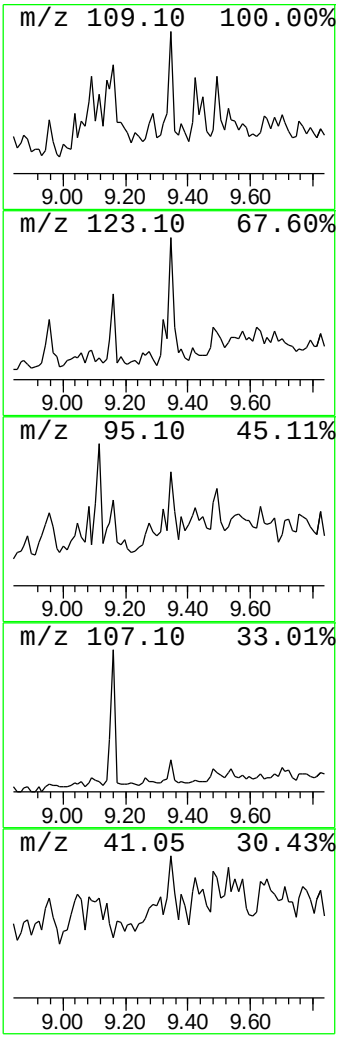
****

Peak Number 6 unknown9.34 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.34	2.06 ng	48291	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[4.3.1.1(3,8)]undecane, ...	180	C12H20O	021898-95-3	35
2	6,6-Dimethylhepta-2,4-diene	124	C9H16	1000195-03-3	30
3	1-Buten-3-yne,4-trimethylsilyl	124	C7H12Si	002696-32-4	30
4	2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	30
5	1,3-Heptadiene, 2,3-dimethyl-	124	C9H16	074779-65-0	27





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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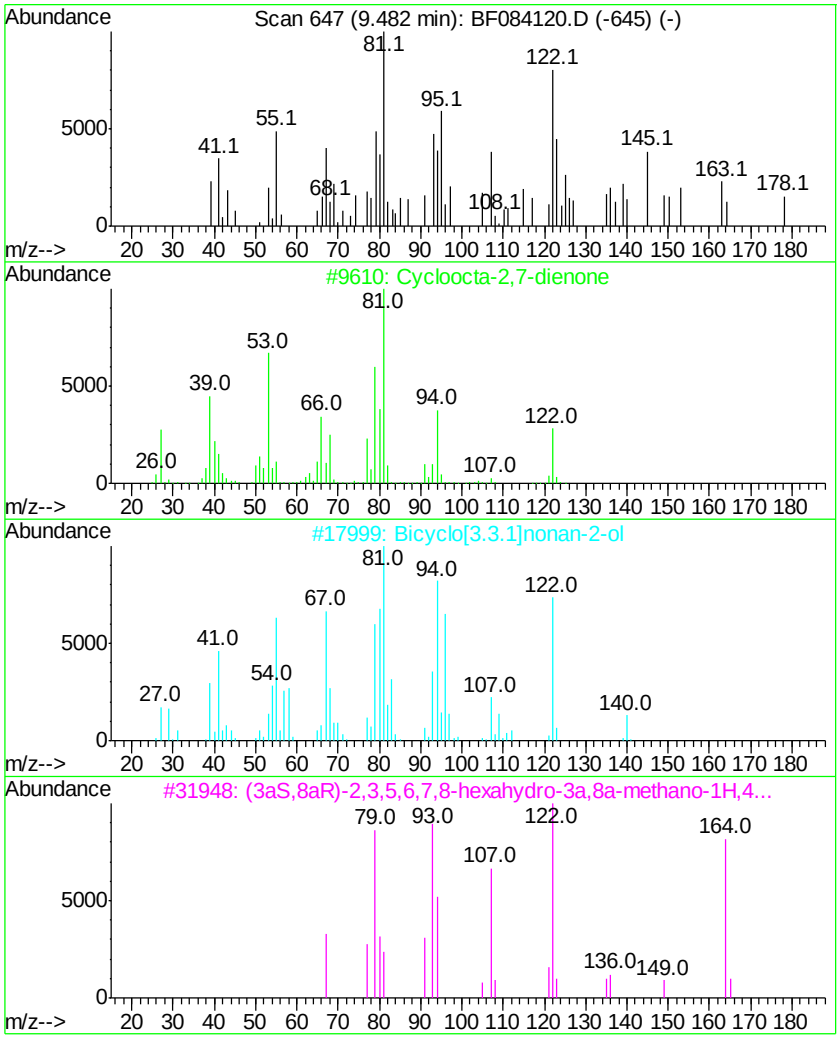
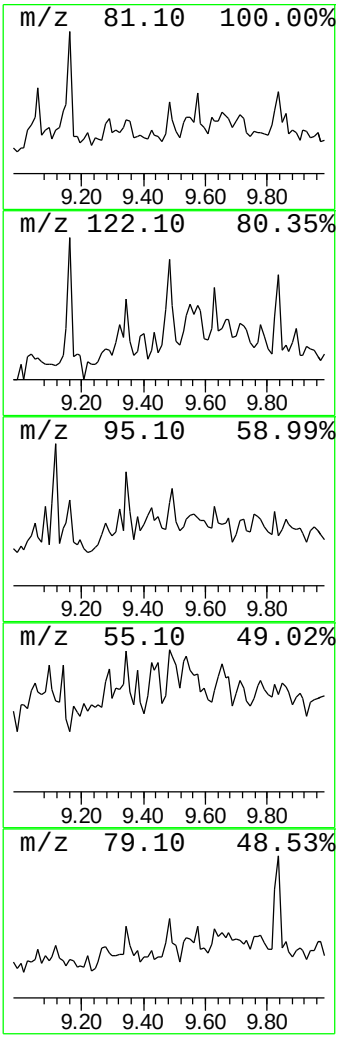
Peak Number 7 unknown9.48 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.48	2.78 ng	65173	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloocta-2,7-dienone	122	C8H10O	1000194-03-3	46
2	Bicyclo[3.3.1]nonan-2-ol	140	C9H16O	002568-14-1	35
3	(3aS,8aR)-2,3,5,6,7,8-hexahydro-...	164	C11H16O	1000145-90-1	30
4	2(1H)-Naphthalenone, 4a,5,6,7,8,...	164	C11H16O	022844-34-4	22
5	Phenol, 2,4-dimethyl-, acetate	164	C10H12O2	000877-53-2	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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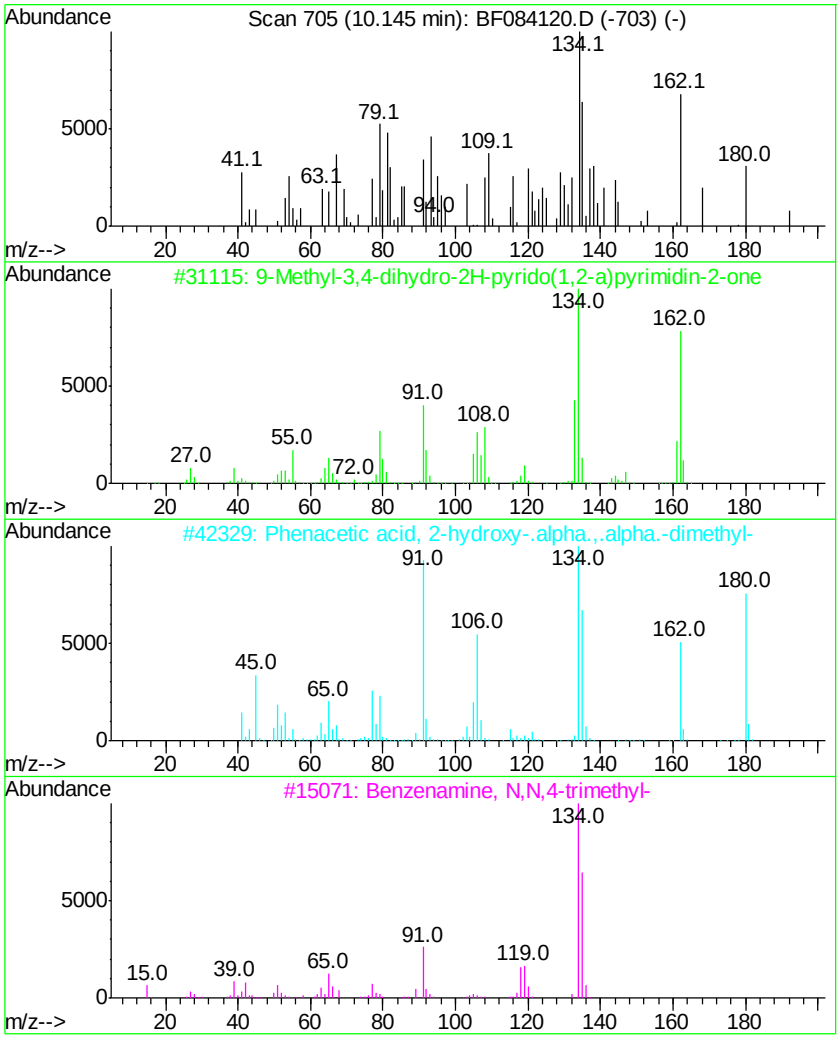
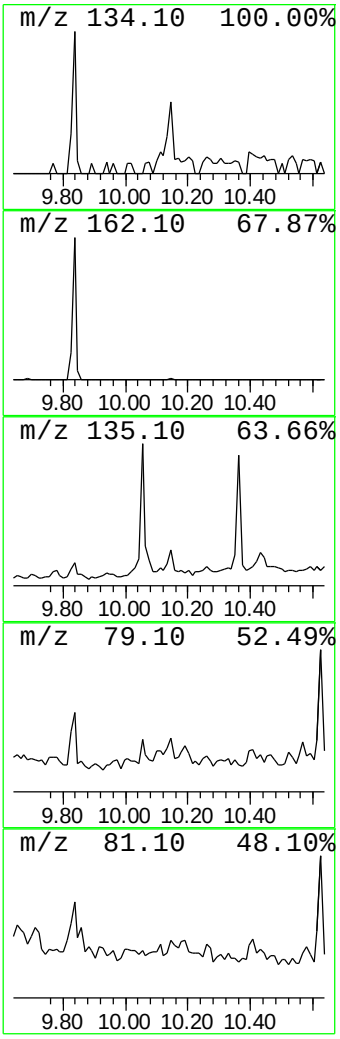
Peak Number 10 unknown10.14 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	2.04 ng	47725	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methyl-3,4-dihydro-2H-pyrido(1...	162	C9H10N2O	061751-44-8	35
2	Phenacetic acid, 2-hydroxy-.alph...	180	C10H12O3	086549-98-6	32
3	Benzenamine, N,N,4-trimethyl-	135	C9H13N	000099-97-8	30
4	Methanamine, N-(phenylmethylene)...	135	C8H9NO	003376-23-6	27
5	Naphthalene, 1,2,3,4-tetrahydro-...	162	C11H14O	001730-48-9	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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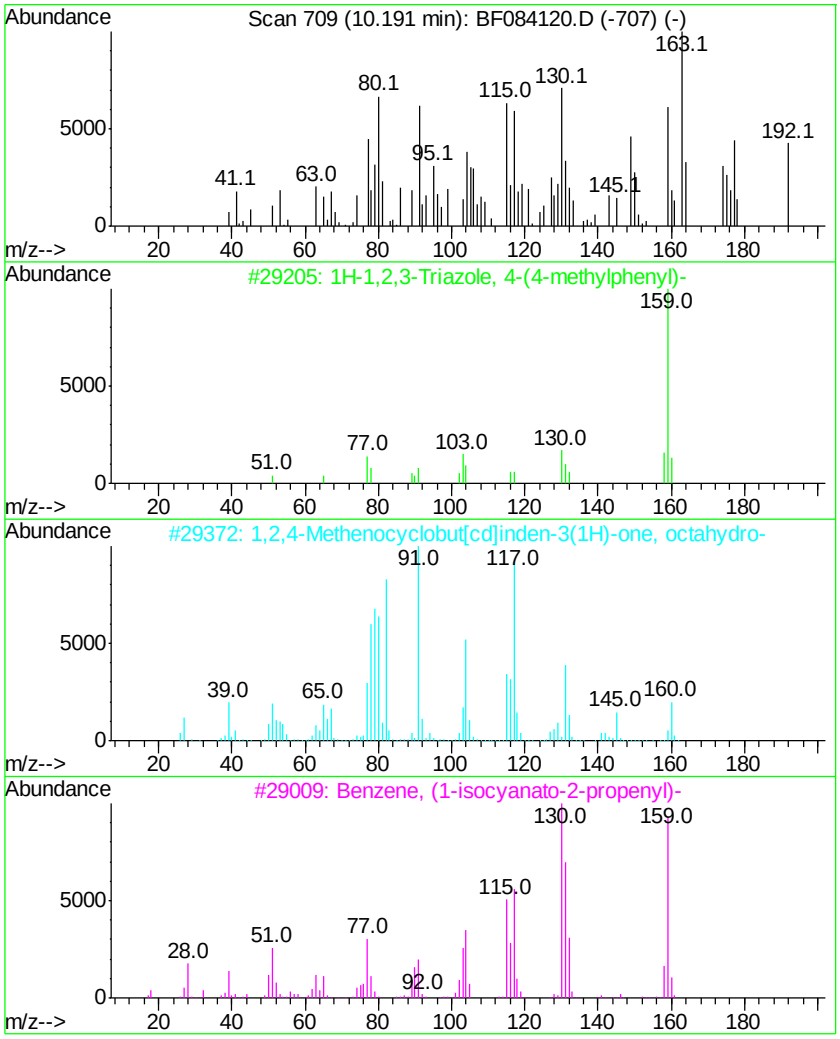
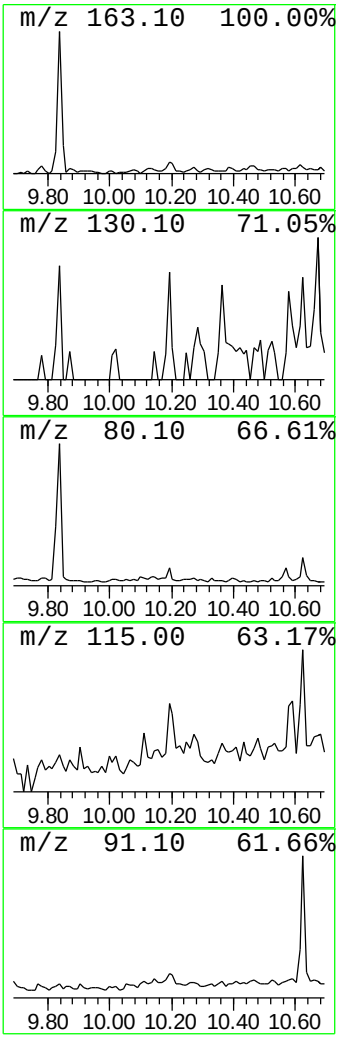
Peak Number 11 unknown10.19 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	3.65 ng	85362	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,2,3-Triazole, 4-(4-methylph...	159	C9H9N3	005301-96-2	35
2	1,2,4-Methenocyclobut[cd]inden-3...	160	C11H12O	061109-83-9	25
3	Benzene, (1-isocyanato-2-propenyl)-	159	C10H9NO	055887-59-7	22
4	4-Benzyl-isoxazolidine	163	C10H13NO	1000186-97-4	18
5	trans-2-Phenyl-1-cyclohexanol	176	C12H16O	002362-61-0	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
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Instrument : BNA_F
ClientSampleId : LIP-22-122315

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

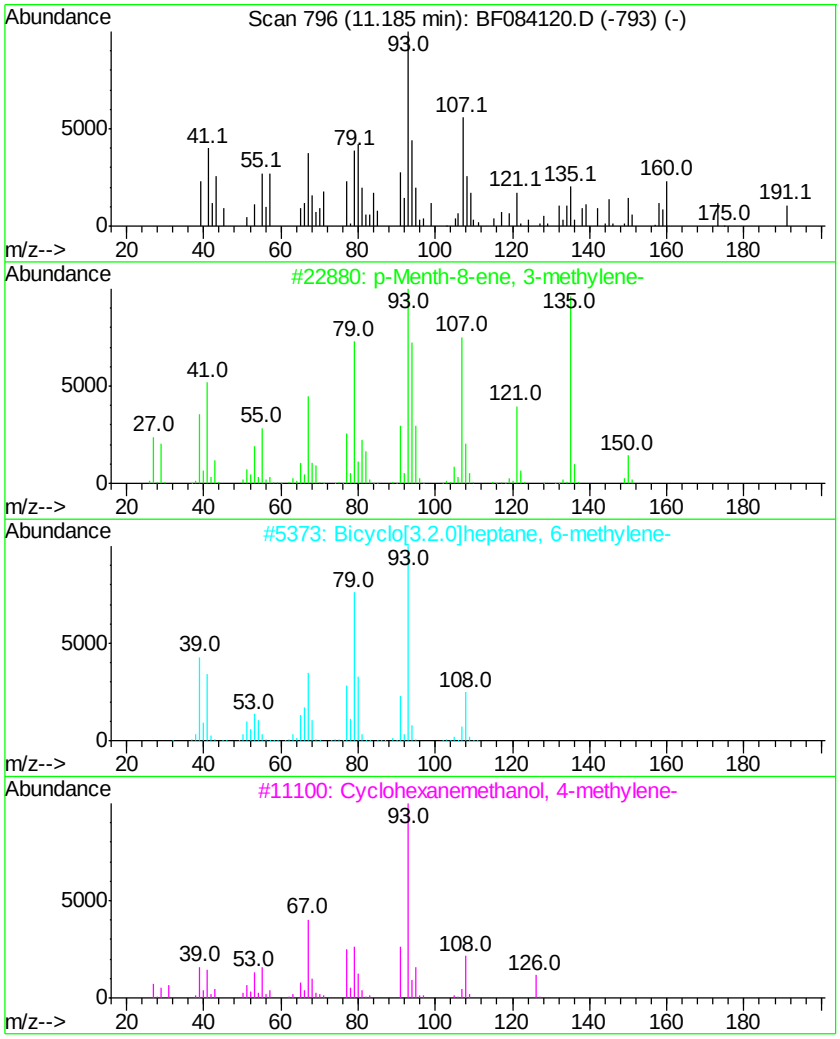
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

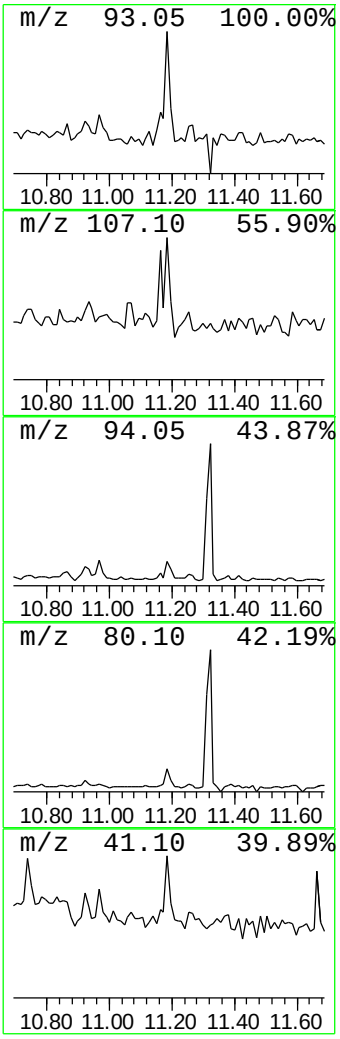
****

Peak Number 13 unknown11.19 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.58 ng	52807	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Menth-8-ene, 3-methylene-	150	C11H18	1000151-25-7	49
2	Bicyclo[3.2.0]heptane, 6-methylene-	108	C8H12	003642-22-6	35
3	Cyclohexanemethanol, 4-methylene-	126	C8H14O	001004-24-6	35
4	2,6,9,11-Dodecatetraenal, 2,6,10...	218	C15H22O	017909-77-2	35
5	1,6-Octadien-3-ol, 3,7-dimethyl-...	273	C17H23NO2	007149-26-0	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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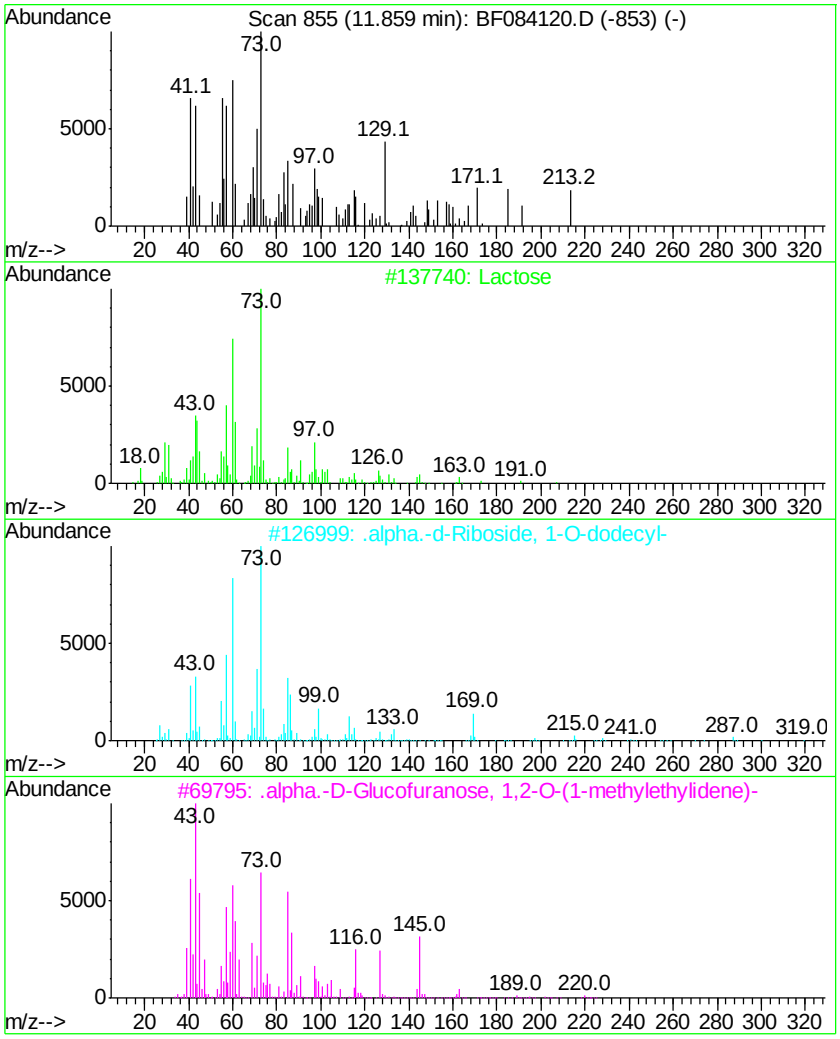
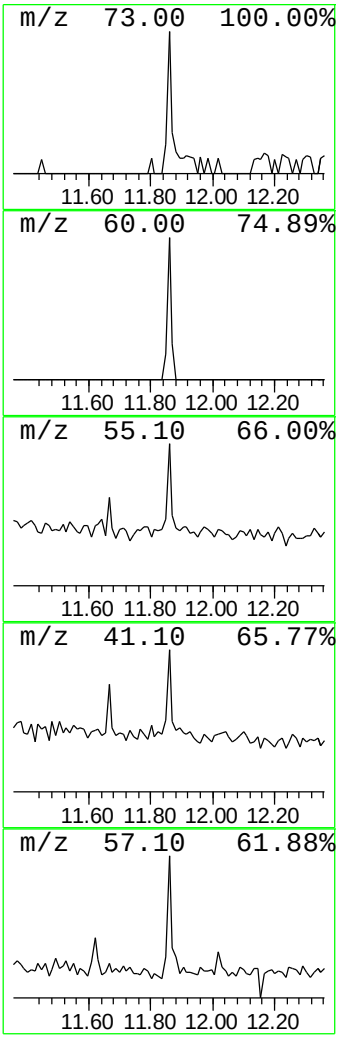
Peak Number 14 unknown11.86 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.60 ng	53177	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lactose	342	C12H22O11	000063-42-3	43
2	.alpha.-d-Riboside, 1-O-dodecyl-	318	C17H34O5	1000154-76-8	38
3	.alpha.-D-Glucofuranose, 1,2-O-(...	220	C9H16O6	018549-40-1	27
4	Decane	142	C10H22	000124-18-5	11
5	Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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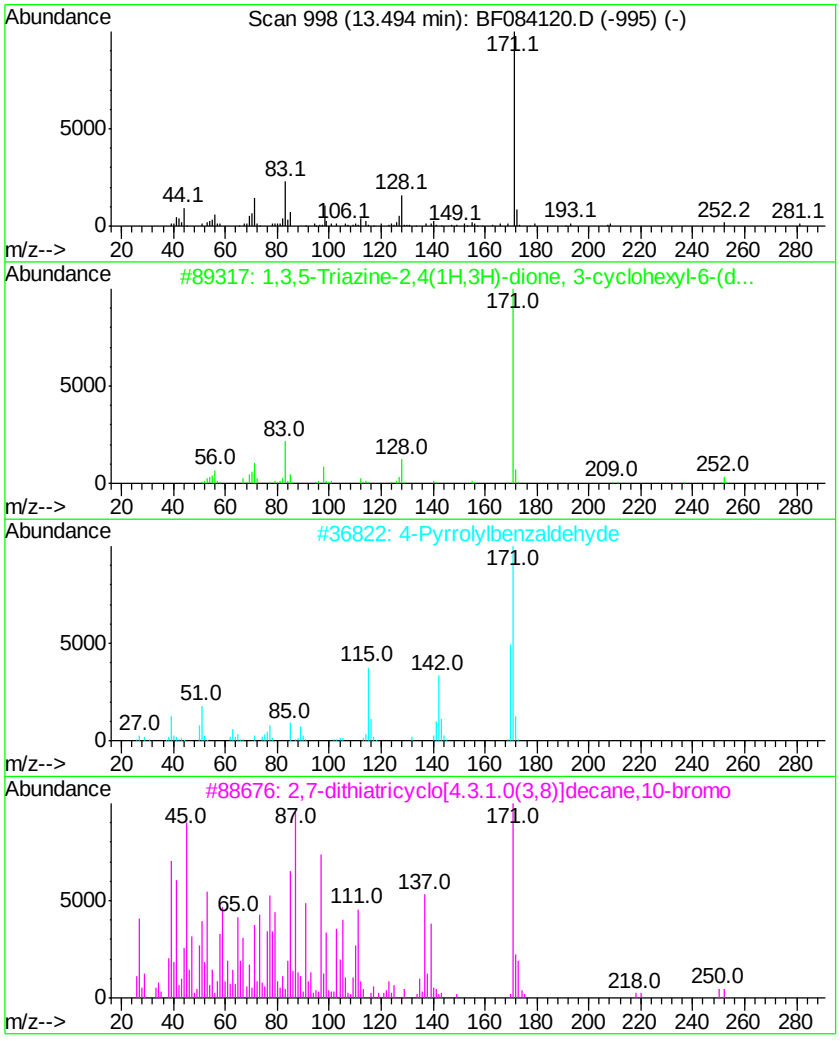
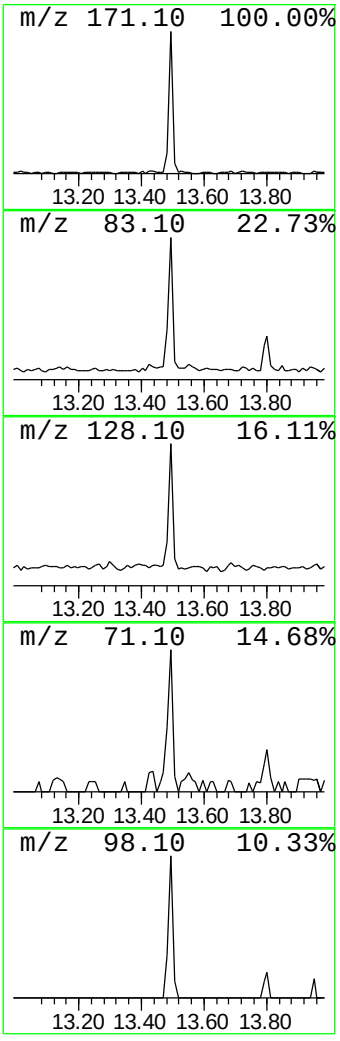
Peak Number 15 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	4.98 ng	81940	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	81
2	4-Pyrrolylbenzaldehyde	171	C11H9NO	023351-05-5	47
3	2,7-dithiatricyclo[4.3.1.0(3,8)]...	250	C8H11BrS2	1000197-96-2	43
4	Quinoline, 2,3,4-trimethyl-	171	C12H13N	002437-72-1	40
5	Benzoic acid, 2,6-difluoro-4-met...	202	C9H8F2O3	084937-82-6	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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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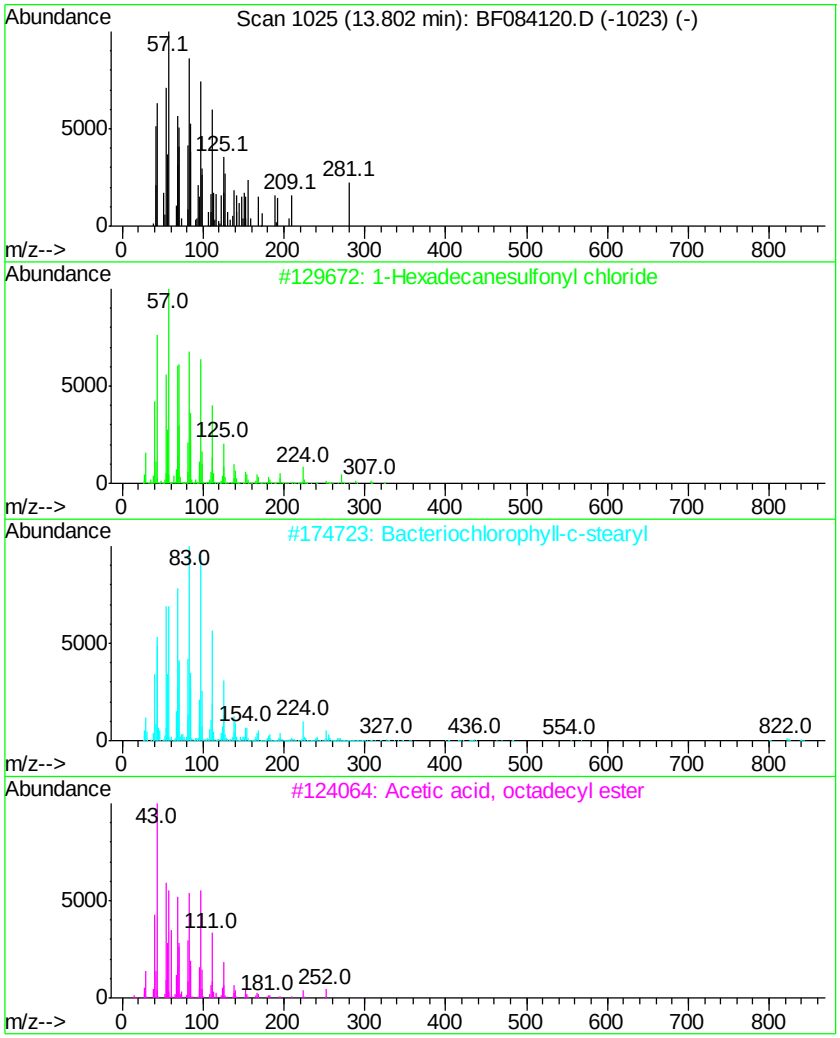
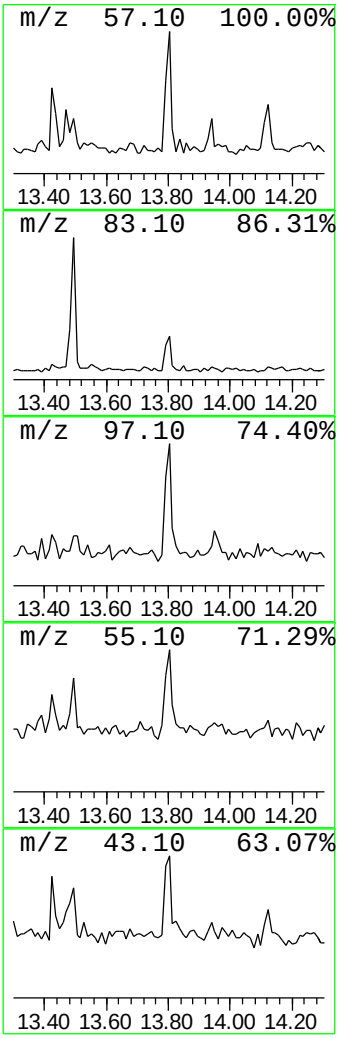
Peak Number 16 1-Hexadecanesulfonyl chloride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.12 ng	51345	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	72
2	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	58
3	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	58
4	Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	52
5	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122415\
Data File : BF084120.D
Acq On : 25 Dec 2015 10:43
Operator : UM/SJ
Sample : G4951-13
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LIP-22-122315

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	7.9	ng	112650	1	6.80	286754	20.0
unknown8.02	8.02	3.0	ng	58835	2	8.09	396856	20.0
unknown8.96	8.96	2.0	ng	40178	2	8.09	396856	20.0
unknown9.34	9.34	2.1	ng	48291	3	9.84	468351	20.0
unknown9.48	9.48	2.8	ng	65173	3	9.84	468351	20.0
unknown10.14	10.14	2.0	ng	47725	3	9.84	468351	20.0
unknown10.19	10.19	3.6	ng	85362	3	9.84	468351	20.0
unknown11.19	11.19	2.6	ng	52807	4	11.32	408901	20.0
unknown11.86	11.86	2.6	ng	53177	4	11.32	408901	20.0
1,3,5-Triazine-2,...	13.49	5.0	ng	81940	5	13.96	329141	20.0
1-Hexadecanesulfo...	13.80	3.1	ng	51345	5	13.96	329141	20.0