LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

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-BF102116.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	5.046	235	237	243	rBV	305360	446588	6.06%	0.818%
2	5.137	243	245	253	rVB	105481	184737	2.51%	0.338%
3	5.457	271	273	276	rBV	2423015	2737071	37.17%	5.011%
4	6.486	361	363	372	rBV	1824196	1936588	26.30%	3.546%
5	6.623	372	375	378	rBV	5055218	5221849	70.91%	9.561%
6	6.852	393	395	400	rBV	1498021	1583670	21.51%	2.900%
7	7.012	406	409	411	rBV	5084709	5098357	69.24%	9.335%
8	7.263	429	431	440	rVB	83523	174182	2.37%	0.319%
9	7.423	441	445	447	rBV	3656348	4431344	60.18%	8.113%
10	7.515	451	453	457	rVB	44877	98949	1.34%	0.181%
11	8.143	505	508	510	rBV	1812852	2088945	28.37%	3.825%
12	8.715	555	558	562	rBV2	44409	100611	1.37%	0.184%
13	9.218	599	602	605	rBV	6284696	7363575	100.00%	13.482%
14	9.606	634	636	639	rBV	427158	564712	7.67%	1.034%
15	9.663	639	641	644	rBV	82411	112975	1.53%	0.207%
16	9.892	658	661	664	rBV	2391567	2275140	30.90%	4.166%
17	10.109	678	680	683	rBV	160515	165025	2.24%	0.302%
18	10.201	685	688	689	rBV	51548	107512	1.46%	0.197%
19	10.281	693	695	698	rVV2	89218	123983	1.68%	0.227%
20	10.406	705	706	709	rBV2	79952	104306	1.42%	0.191%
21	10.681	727	730	733	rBV2	2998142	4588413	62.31%	8.401%
22	10.806	738	741	745	rVB4	62378	155374	2.11%	0.284%
23	10.898	747	749	751	rVB2	82449	99110	1.35%	0.181%
24	11.058	760	763	768	rBV2	492278	759430	10.31%	1.390%
25	11.252	776	780	781	rBV2	62748	97450	1.32%	0.178%
26	11.332	786	787	789	rBV	53474	83360	1.13%	0.153%
27	11.378	789	791	794	rBV	2208704	2067632	28.08%	3.786%
28	11.606	809	811	816	rBV	354684	437628	5.94%	0.801%
29	11.926	836	839	842	rBV2	423464	680515	9.24%	1.246%
30	12.429	881	883	886	rVB2	205325	230580	3.13%	0.422%
31	12.852	918	920	928	rVB	301788	424260	5.76%	0.777%
32	12.978	928	931	933	rBV	4796632	7120352	96.70%	13.037%
33	13.869	1007	1009	1013	rVB	72946	112218	1.52%	0.205%
34	14.018	1019	1022	1024	rBV	1304819	1418465	19.26%	2.597%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

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-BF102116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.447	1144	1147	1155	rBV	743370	1073611	14.58%	1.966%
36	16.133	1204	1207	1213	rBV2	51286	115439	1.57%	0.211%
37	16.315	1218	1223	1231	rBV4	87048	233992	3.18%	0.428%

Sum of corrected areas: 54617948

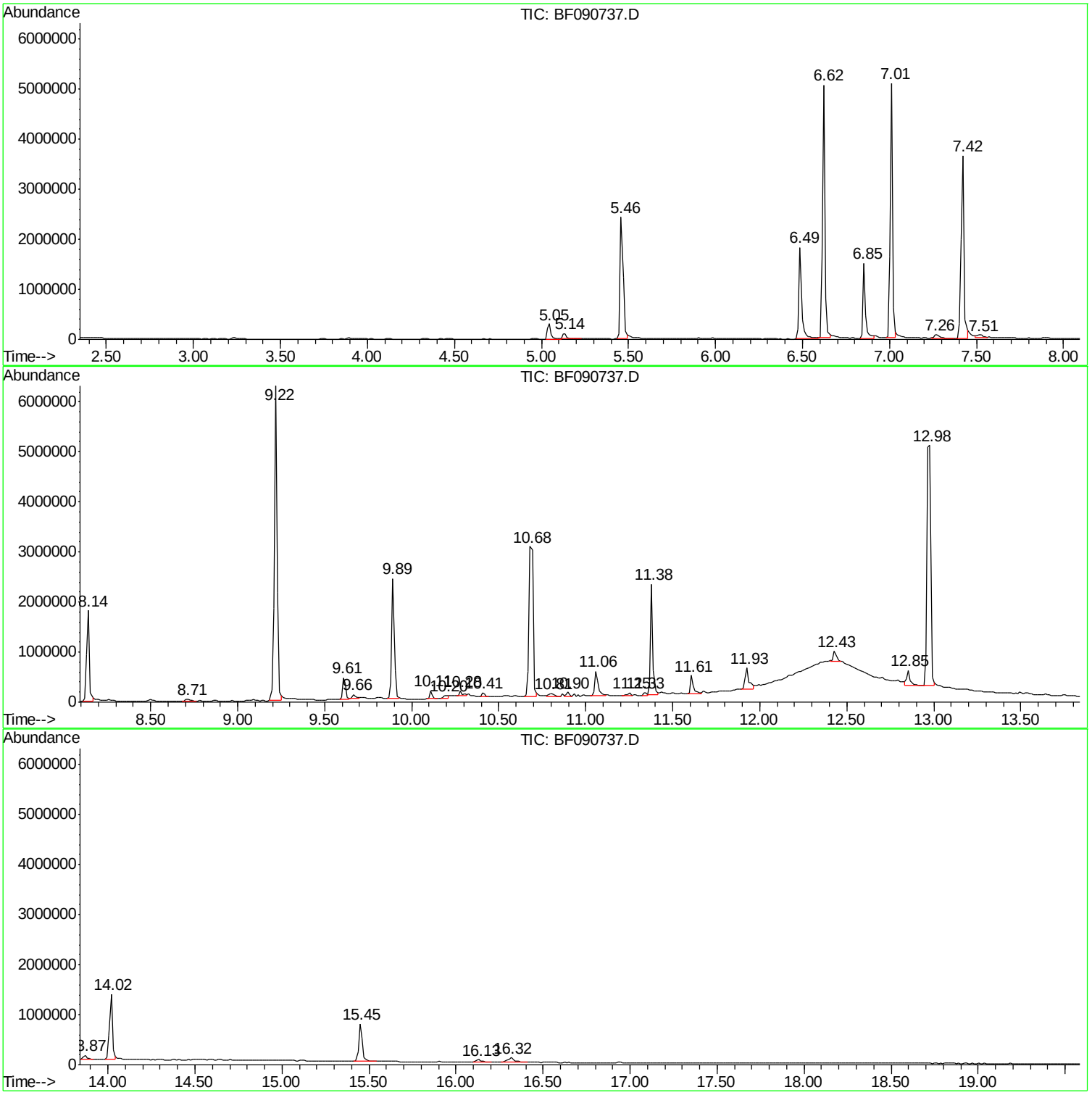
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

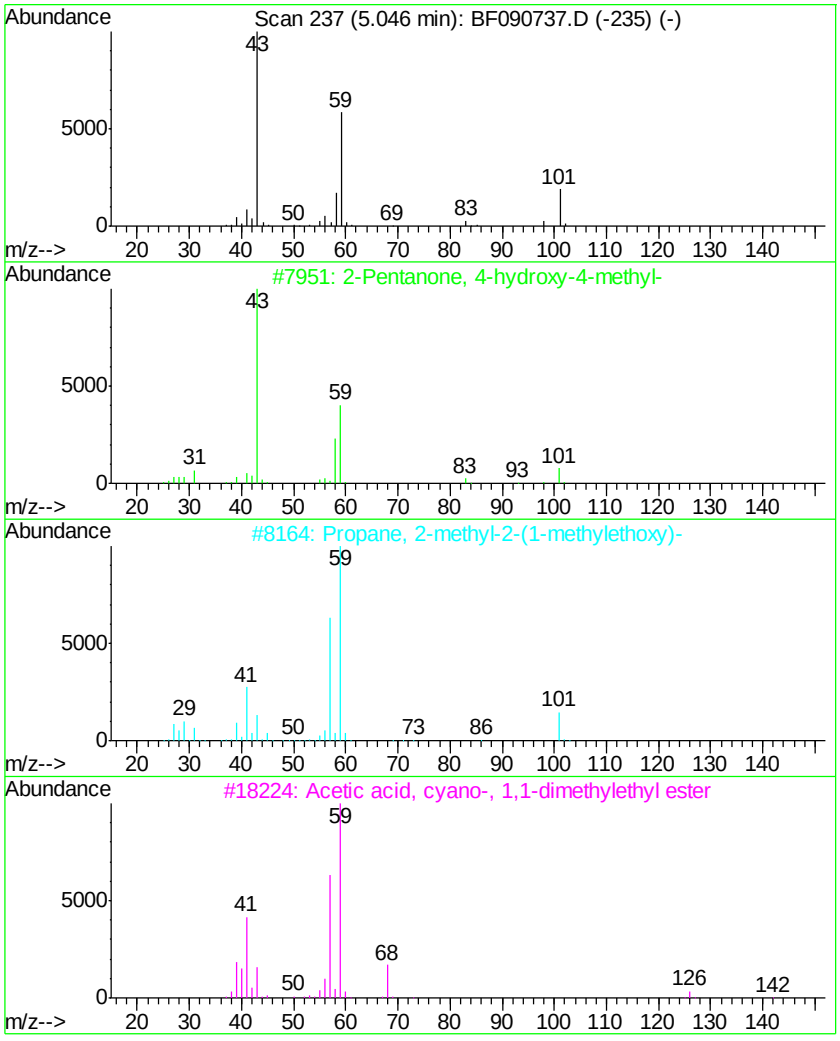
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

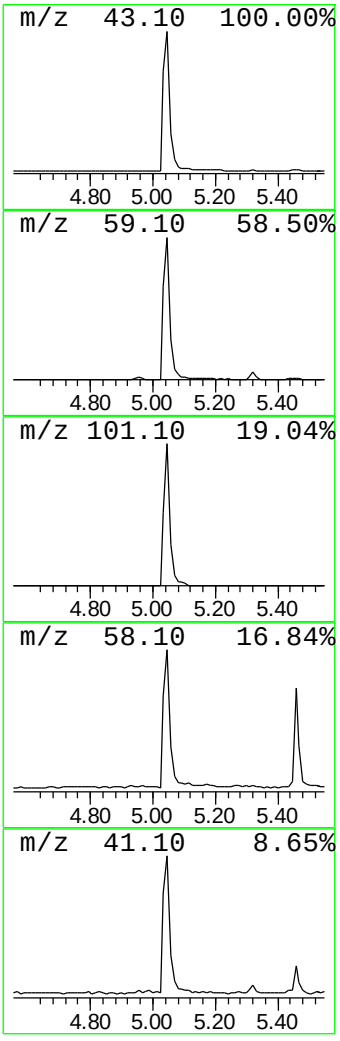
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	5.64 ng	446588	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

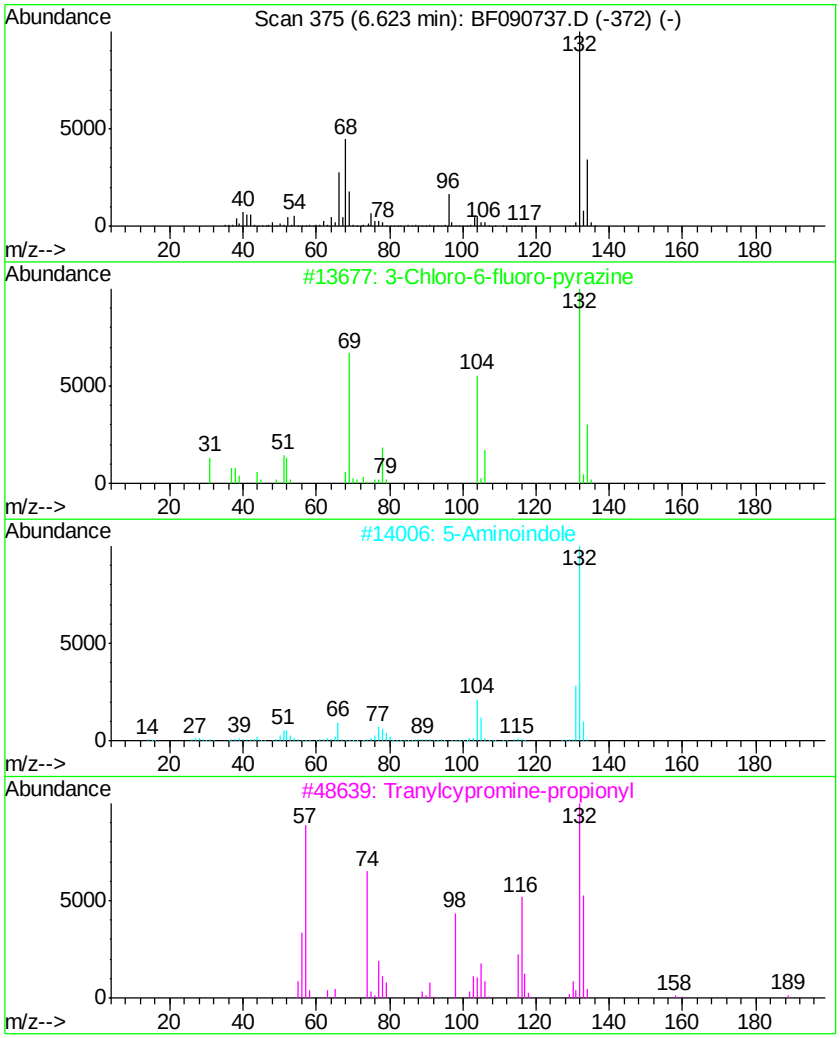
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

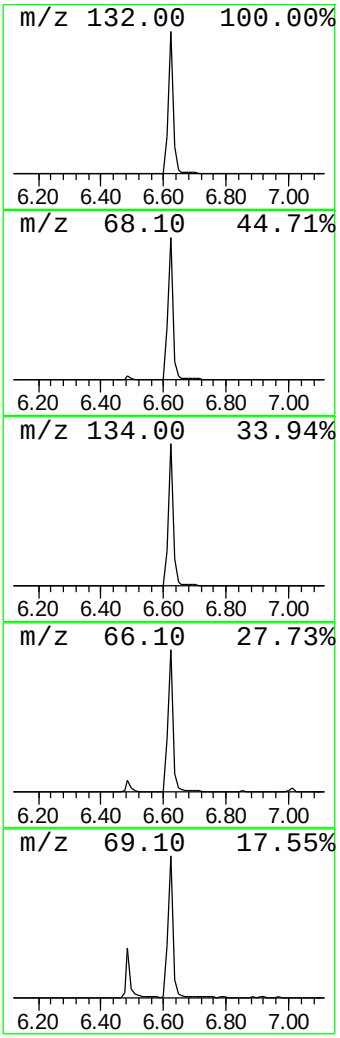
****

Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	65.95 ng	5221850	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

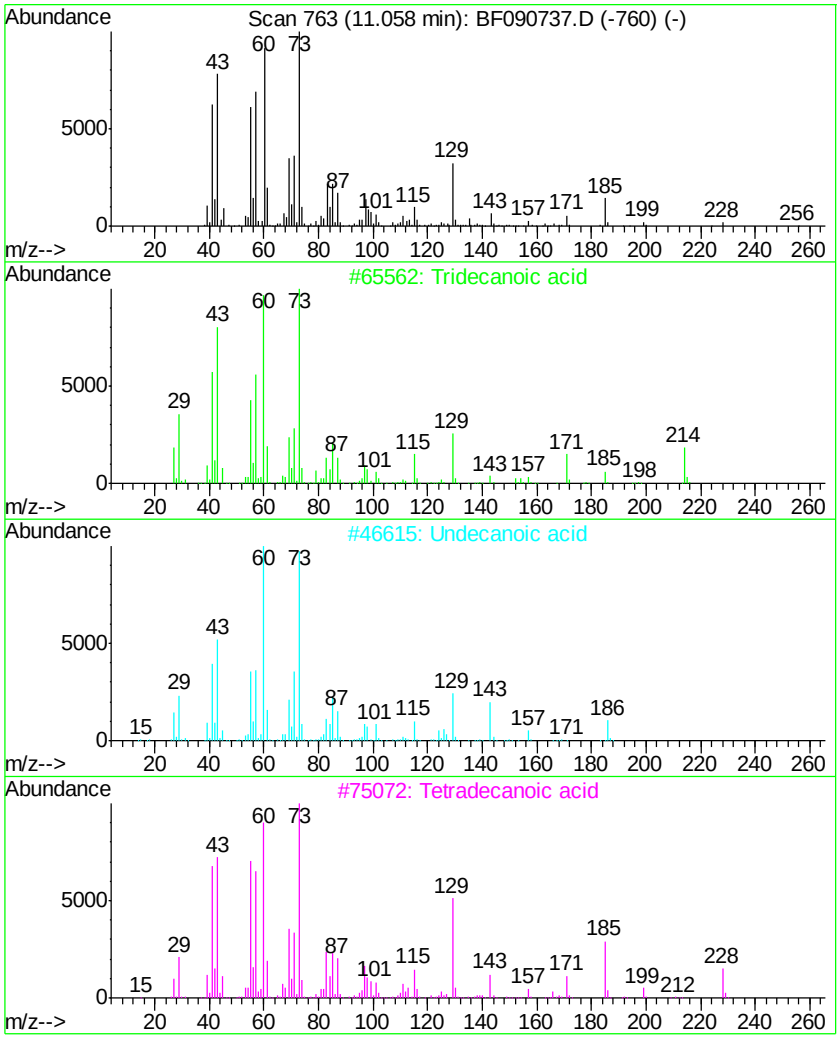
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

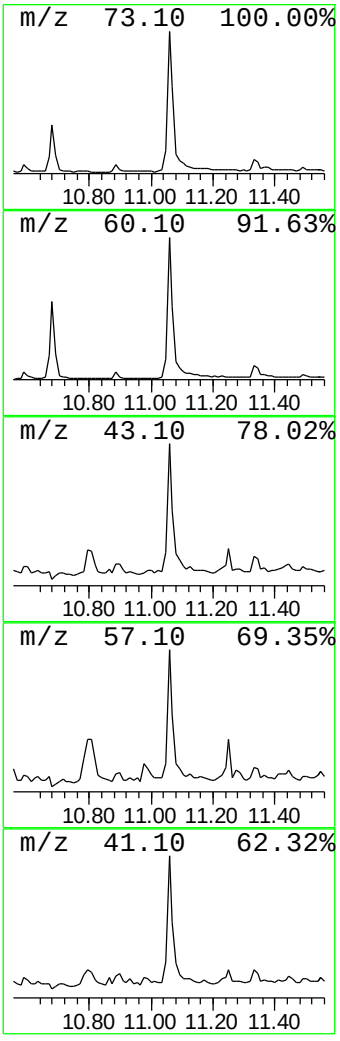
****

Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	7.35 ng	759430	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	86
2	Undecanoic acid	186	C11H22O2	000112-37-8	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	60
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

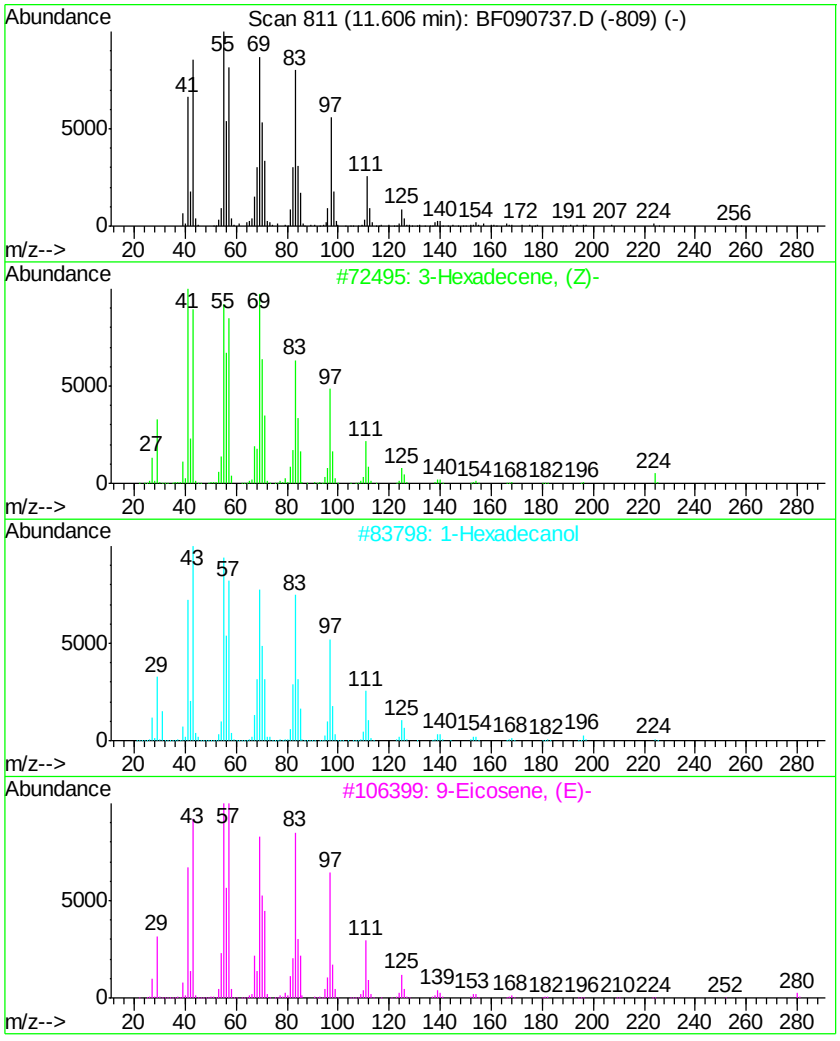
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

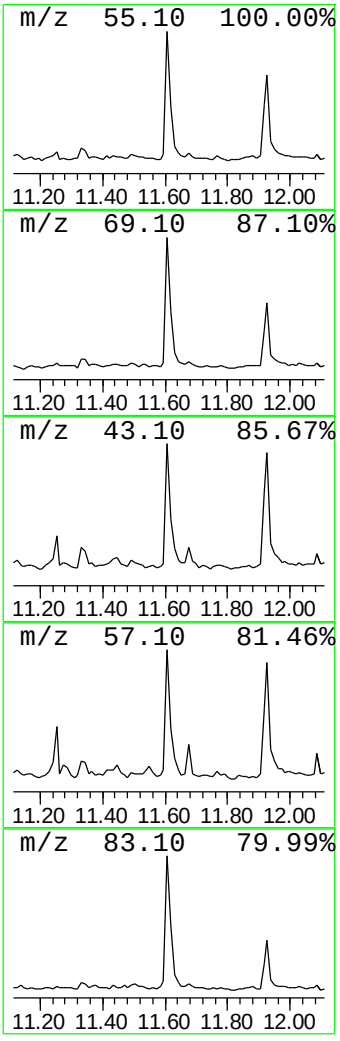
****

Peak Number 6 3-Hexadecene, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	4.23 ng	437628	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexadecene, (Z)-	224	C16H32	034303-81-6	98
2	1-Hexadecanol	242	C16H34O	036653-82-4	94
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	91





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Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

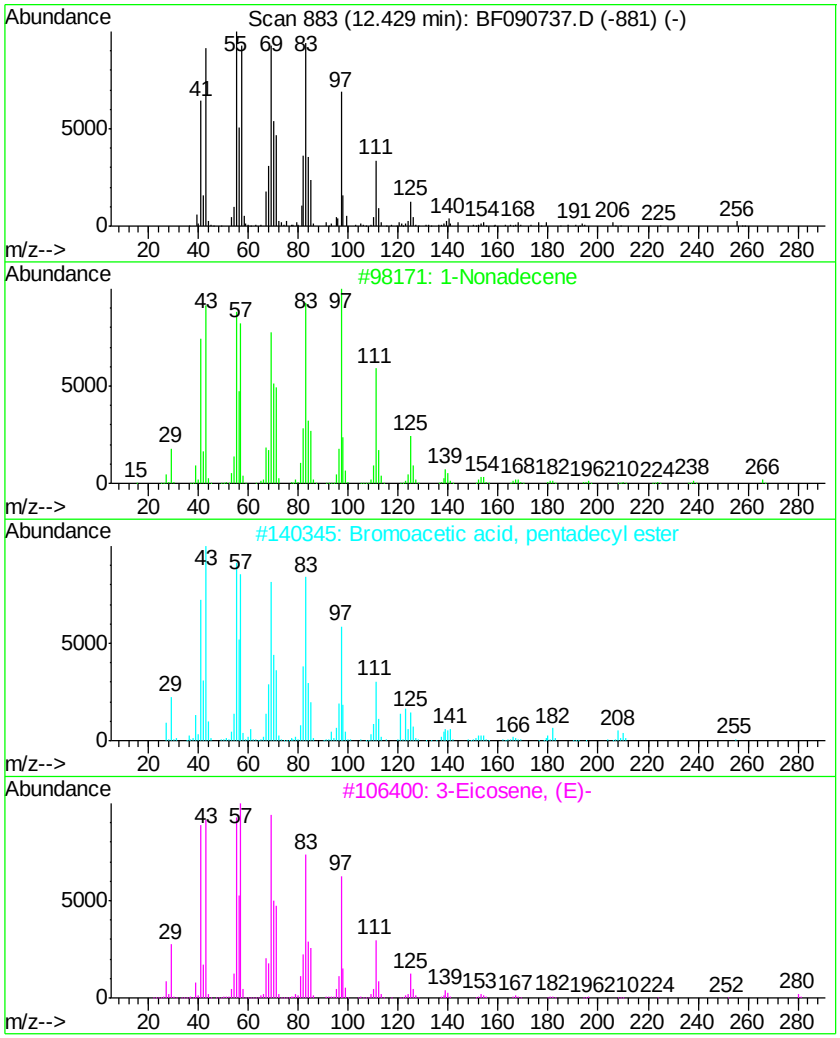
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

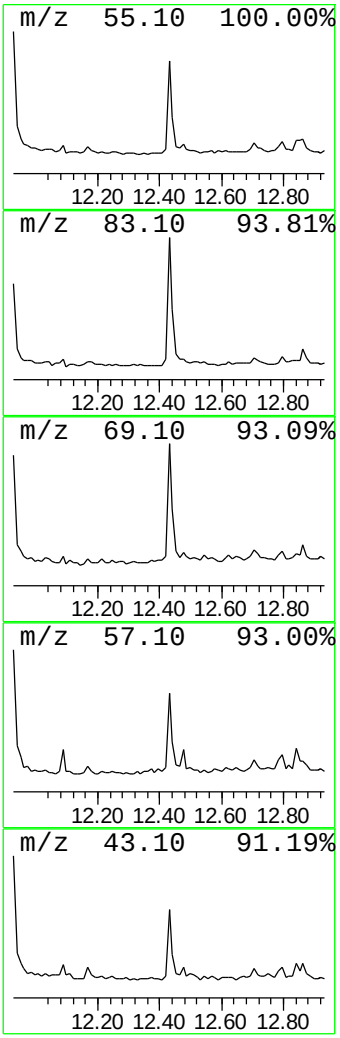
****

Peak Number 8 1-Nonadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	2.23 ng	230580	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91





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Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

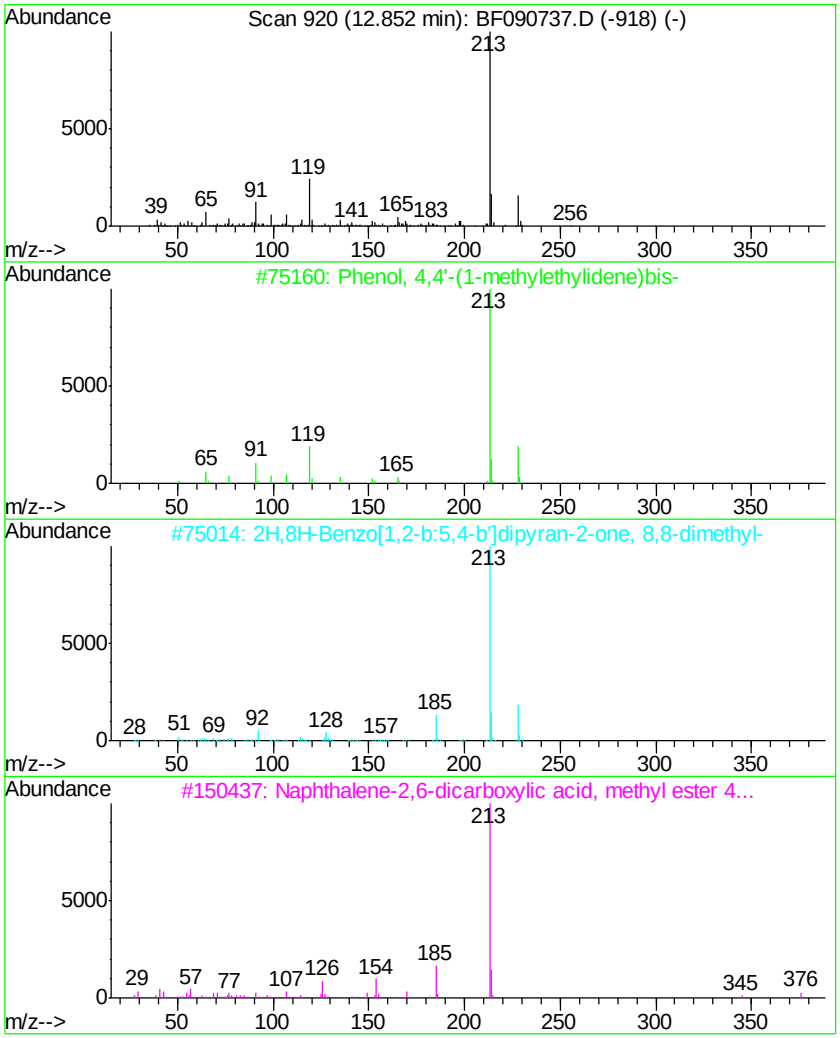
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

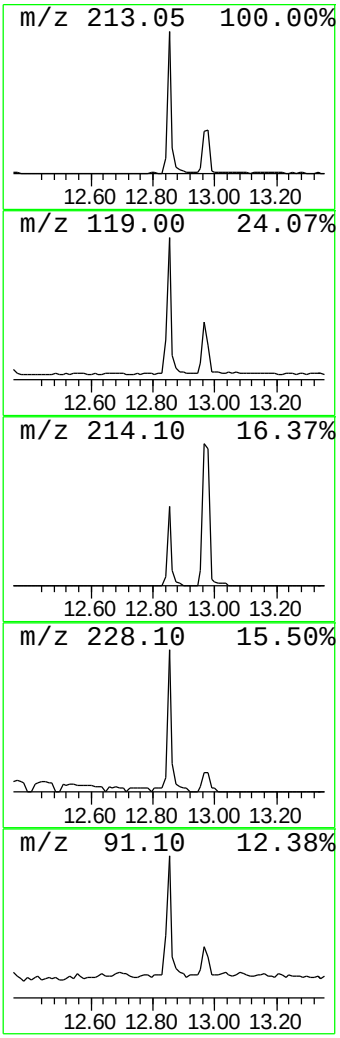
****

Peak Number 9 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	5.98 ng	424260	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53
3	Naphthalene-2,6-dicarboxylic aci...	376	C24H24O4	1000189-60-8	50
4	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	42
5	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	40





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Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

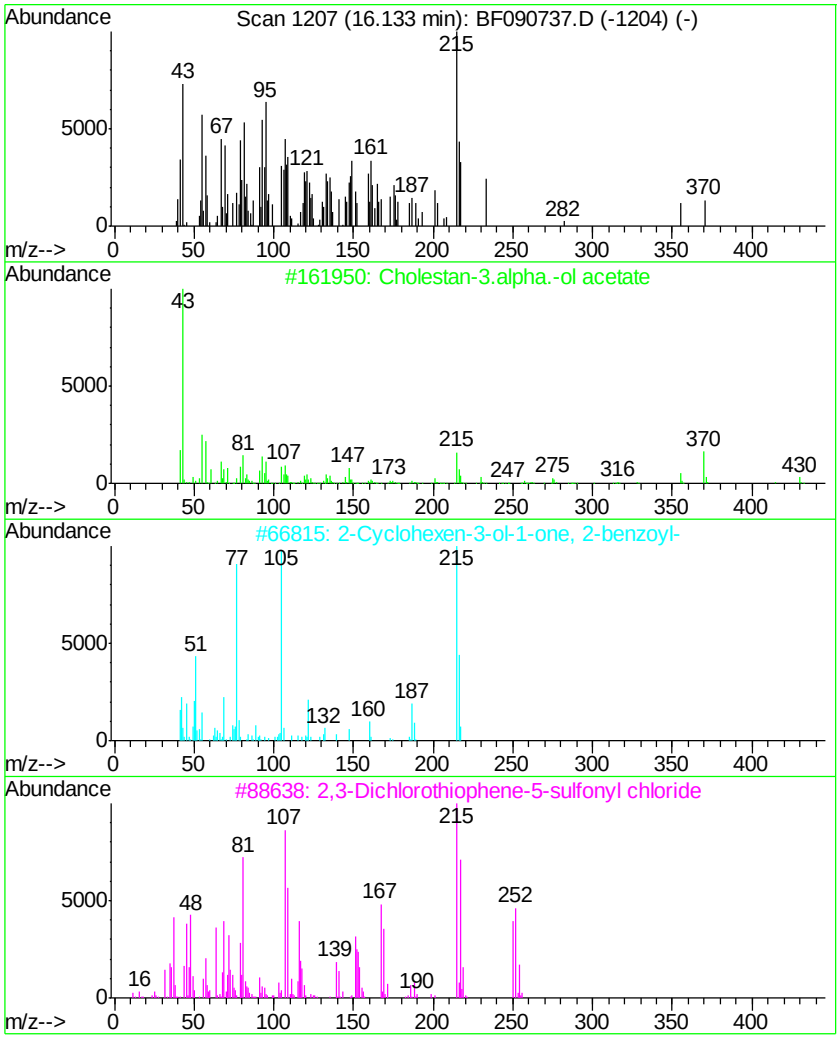
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

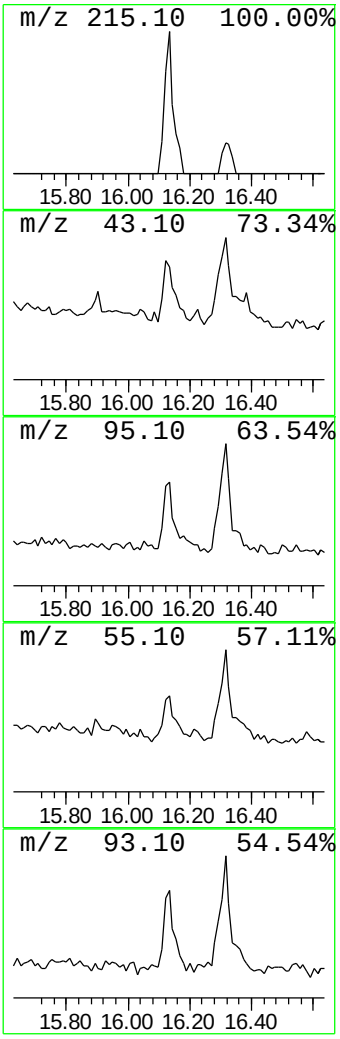
****

Peak Number 10 unknown16.13 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.15 ng	115439	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3.alpha.-ol acetate	430	C29H50O2	1000214-83-2	42
2	2-Cyclohexen-3-ol-1-one, 2-benzoyl-	216	C13H12O3	061834-43-3	30
3	2,3-Dichlorothiophene-5-sulfonyl...	250	C4HCl3O2S2	126714-85-0	22
4	1-Cycloheptene-3-carboxamide, N-...	215	C14H17NO	1000159-24-4	22
5	2-Norbornanamine, N-ethyl-3-phenyl-	215	C15H21N	001209-98-9	18





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

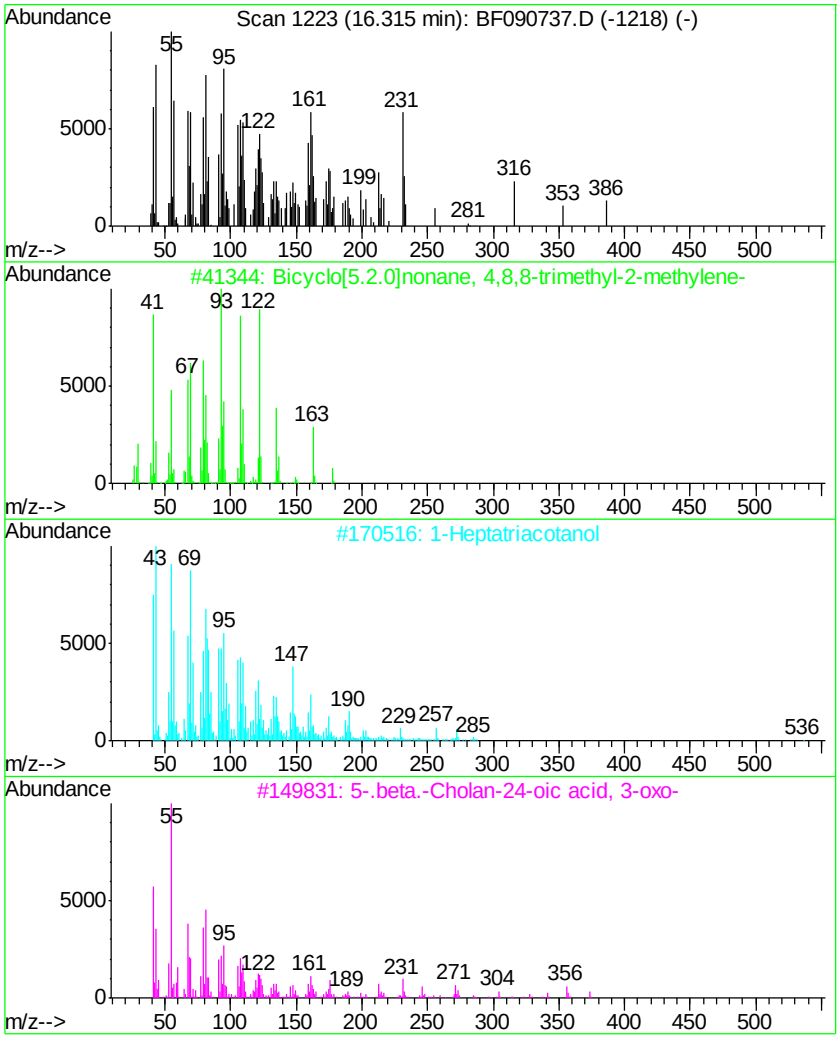
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

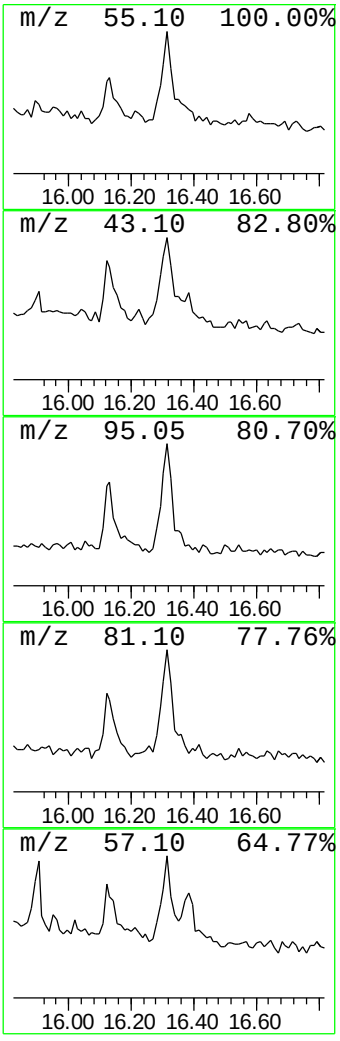
****

Peak Number 11 unknown16.32 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	4.36 ng	233992	Perylene-d12	15.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[5.2.0]nonane, 4,8,8-trim...	178	C13H22	1000149-59-1	43
2	1-Heptatriacotanol	537	C37H76O	105794-58-9	38
3	5-.beta.-Cholan-24-oic acid, 3-oxo-	374	C24H38O3	001553-56-6	38
4	3,20-Allopregnanedione	316	C21H32O2	000566-65-4	22
5	Naphtho[2,3-b]furan-9(4H)-one, 4...	232	C15H20O2	015404-32-7	20





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102116\
Data File : BF090737.D
Acq On : 22 Oct 2016 3:44
Operator : UM/SJ
Sample : H5308-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-105S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102116.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...	5.05	5.6	ng	446588	1	6.85	1583670	20.0
unknown6.62	6.62	66.0	ng	5221850	1	6.85	1583670	20.0
Tridecanoic acid	11.06	7.3	ng	759430	4	11.38	2067630	20.0
3-Hexadecene, (Z)-	11.61	4.2	ng	437628	4	11.38	2067630	20.0
1-Nonadecene	12.43	2.2	ng	230580	4	11.38	2067630	20.0
Phenol, 4,4'-(1-m...	12.85	6.0	ng	424260	5	14.02	1418470	20.0
unknown16.13	16.13	2.1	ng	115439	6	15.45	1073610	20.0
unknown16.32	16.32	4.4	ng	233992	6	15.45	1073610	20.0