LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-65-10.0-15.0

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-BF080416.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	4.650	265	268	279	rBV	25764	60175	4.28%	0.609%
2	5.324	325	327	345	rBV	202955	439862	31.29%	4.452%
3	6.982	470	472	479	rBV	103974	281832	20.05%	2.852%
4	7.085	479	481	499	rVB	609430	1014852	72.20%	10.271%
5	7.450	511	513	523	rBV	100907	224406	15.97%	2.271%
6	7.588	523	525	527	rVV	10213	15383	1.09%	0.156%
7	7.679	530	533	557	rVB	616879	886923	63.10%	8.976%
8	8.353	589	592	607	rBV	418727	714041	50.80%	7.227%
9	9.473	687	690	704	rBV	201414	347628	24.73%	3.518%
10	9.713	709	711	714	rVB	15968	20055	1.43%	0.203%
11	11.256	842	846	848	rBV	896326	1405607	100.00%	14.226%
12	11.942	903	906	909	rBV	30784	38107	2.71%	0.386%
13	12.011	909	912	915	rVV	36071	54245	3.86%	0.549%
14	12.068	915	917	920	rVB	177310	212959	15.15%	2.155%
15	12.297	934	937	939	rBV	251285	398598	28.36%	4.034%
16	12.388	942	945	952	rVB	27543	51566	3.67%	0.522%
17	12.811	979	982	984	rBV	26859	33705	2.40%	0.341%
18	12.902	988	990	993	rBV3	16483	27932	1.99%	0.283%
19	13.017	997	1000	1004	rBV	22243	30052	2.14%	0.304%
20	13.154	1010	1012	1014	rVB	23628	29224	2.08%	0.296%
21	13.508	1040	1043	1047	rVB3	7029	16219	1.15%	0.164%
22	13.577	1047	1049	1057	rBV	510777	837306	59.57%	8.474%
23	13.920	1076	1079	1084	rBV	28637	46082	3.28%	0.466%
24	14.377	1115	1119	1124	rBV6	6659	20113	1.43%	0.204%
25	14.651	1141	1143	1144	rBV	13713	17781	1.27%	0.180%
26	14.685	1144	1146	1155	rVB	282140	401535	28.57%	4.064%
27	15.714	1232	1236	1242	rBV	119586	243746	17.34%	2.467%
28	16.663	1316	1319	1320	rBV3	12362	20378	1.45%	0.206%
29	16.800	1328	1331	1340	rBV	134484	261975	18.64%	2.651%
30	17.051	1350	1353	1356	rBV	916085	1136951	80.89%	11.507%
31	18.309	1461	1463	1468	rBV2	56207	76731	5.46%	0.777%
32	18.389	1468	1470	1476	rBV	177374	276442	19.67%	2.798%
33	20.046	1612	1615	1621	rVB	153044	222481	15.83%	2.252%
34	20.892	1685	1689	1696	rVB4	4002	15652	1.11%	0.158%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-65-10.0-15.0

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-BF080416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 9880544

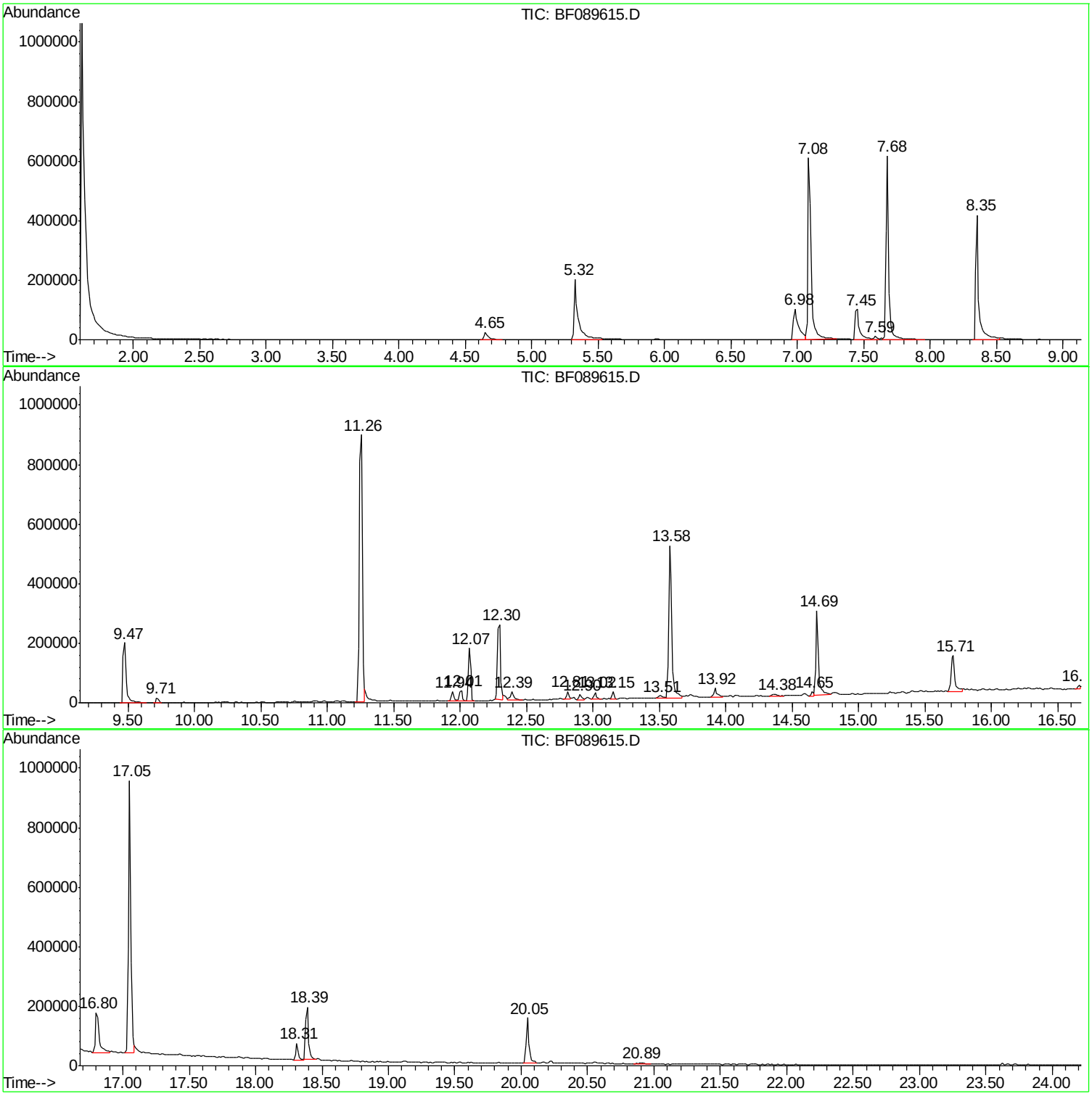
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-65-10.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
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Instrument :
BNA_F
ClientSampleId :
GW-65-10.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

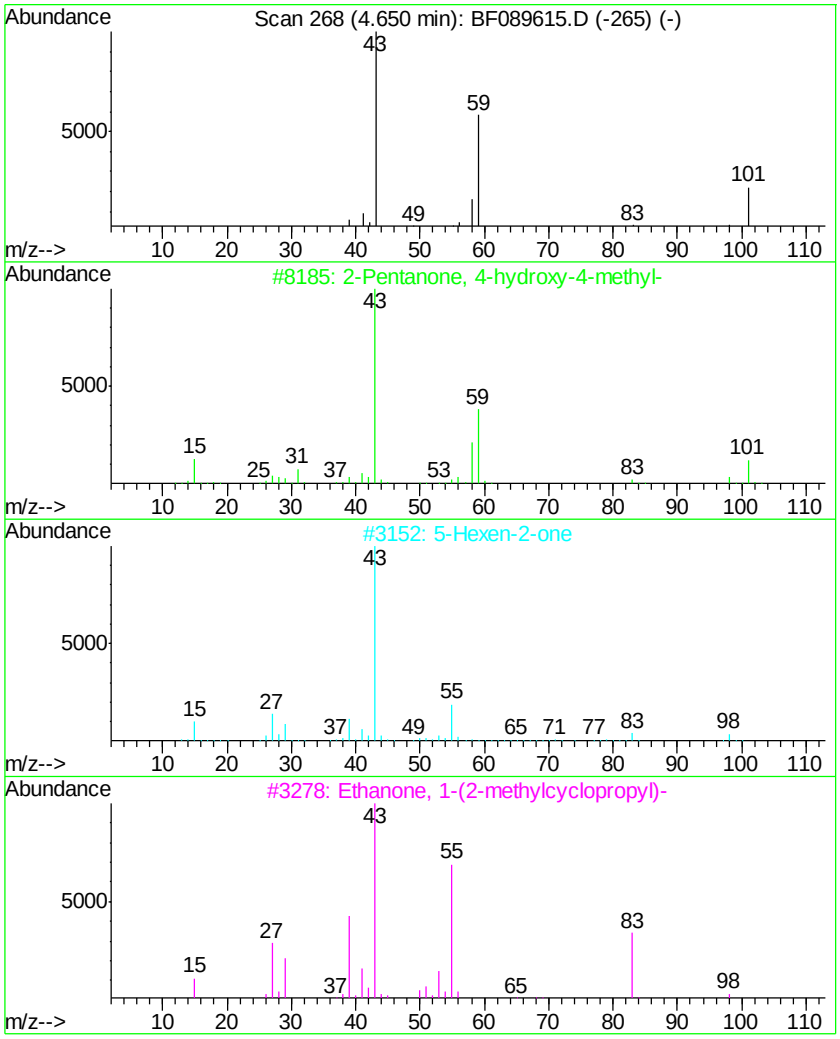
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

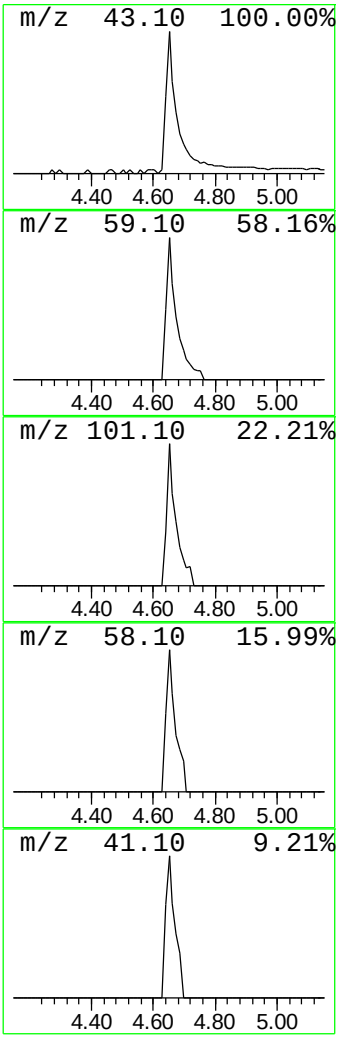
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	5.36 ng	60175	1,4-Dichlorobenzene-d4	7.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	5
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	4





Library Search Compound Report

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Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-65-10.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

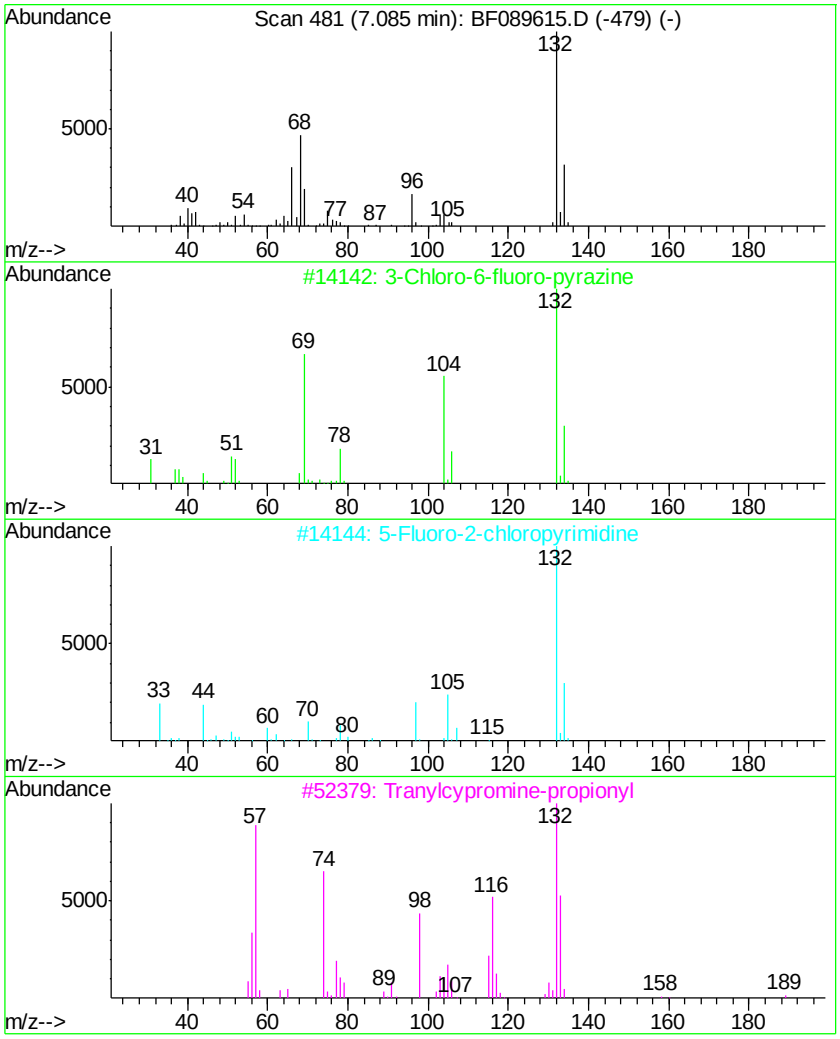
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

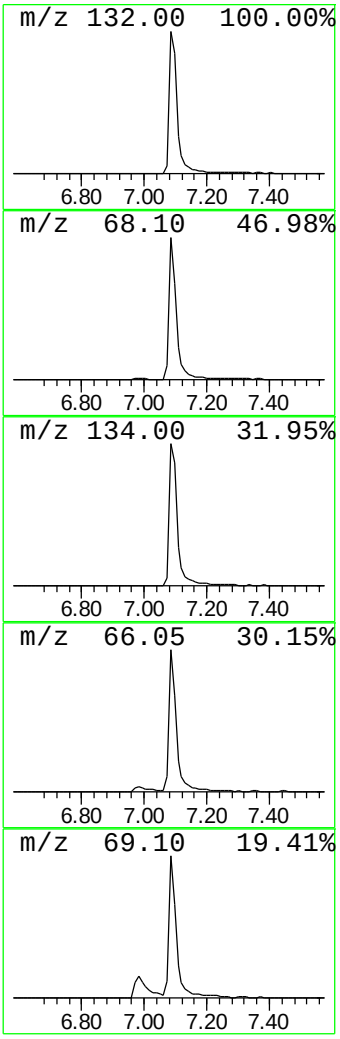
****

Peak Number 2 unknown7.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	90.45 ng	1014850	1,4-Dichlorobenzene-d4	7.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-65-10.0-15.0

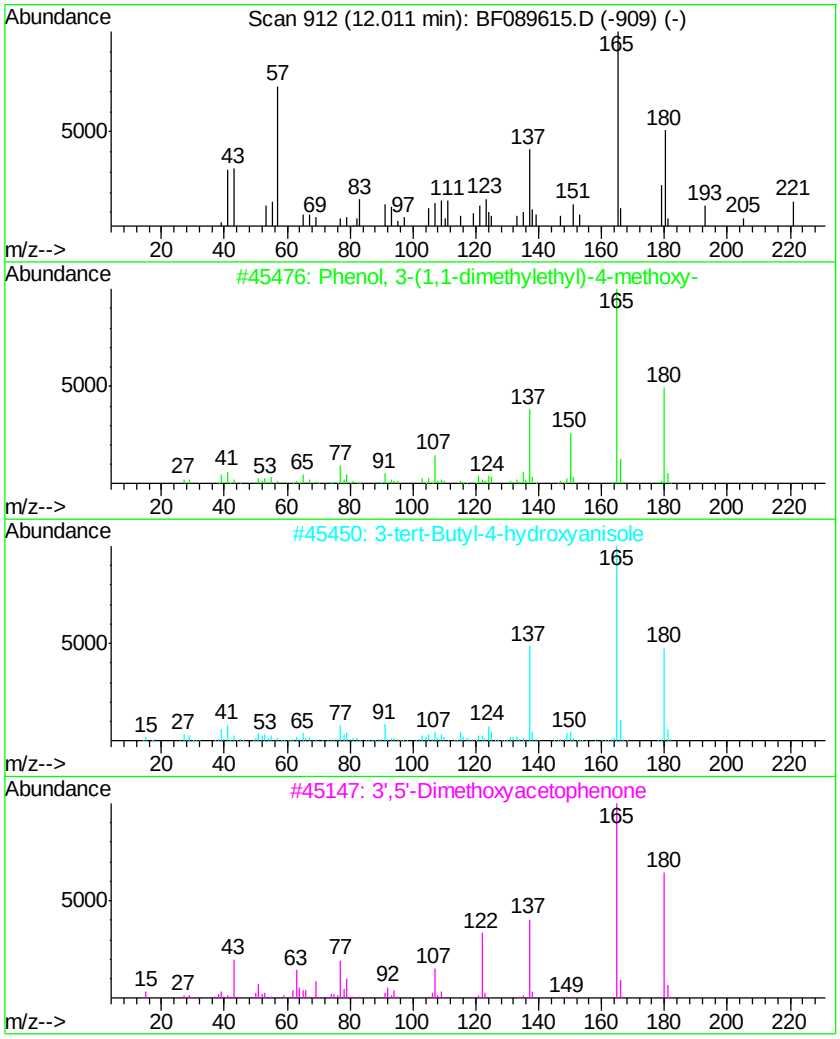
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

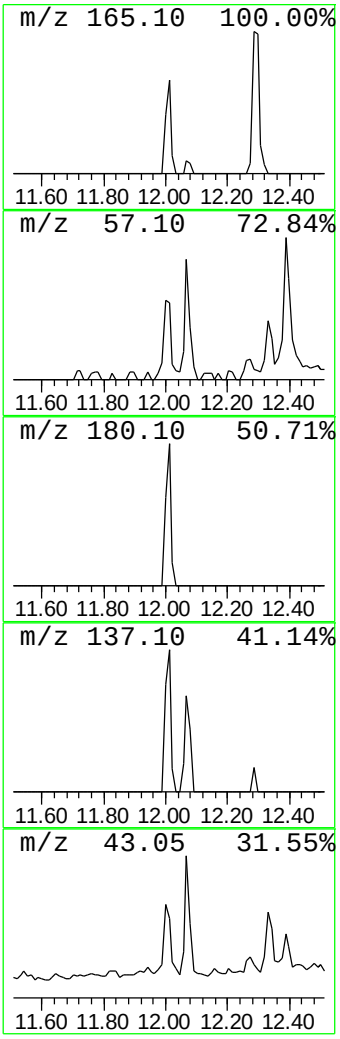
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 3-(1,1-dimethylethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.72 ng	54245	Acenaphthene-d10	12.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	68
2	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	64
3	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	58
4	Thiazolo[5,4-d]pyrimidine, 5-(et...	180	C7H8N4S	019835-21-3	49
5	9H-Fluorene, 9-methyl-	180	C14H12	002523-37-7	47





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
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GW-65-10.0-15.0

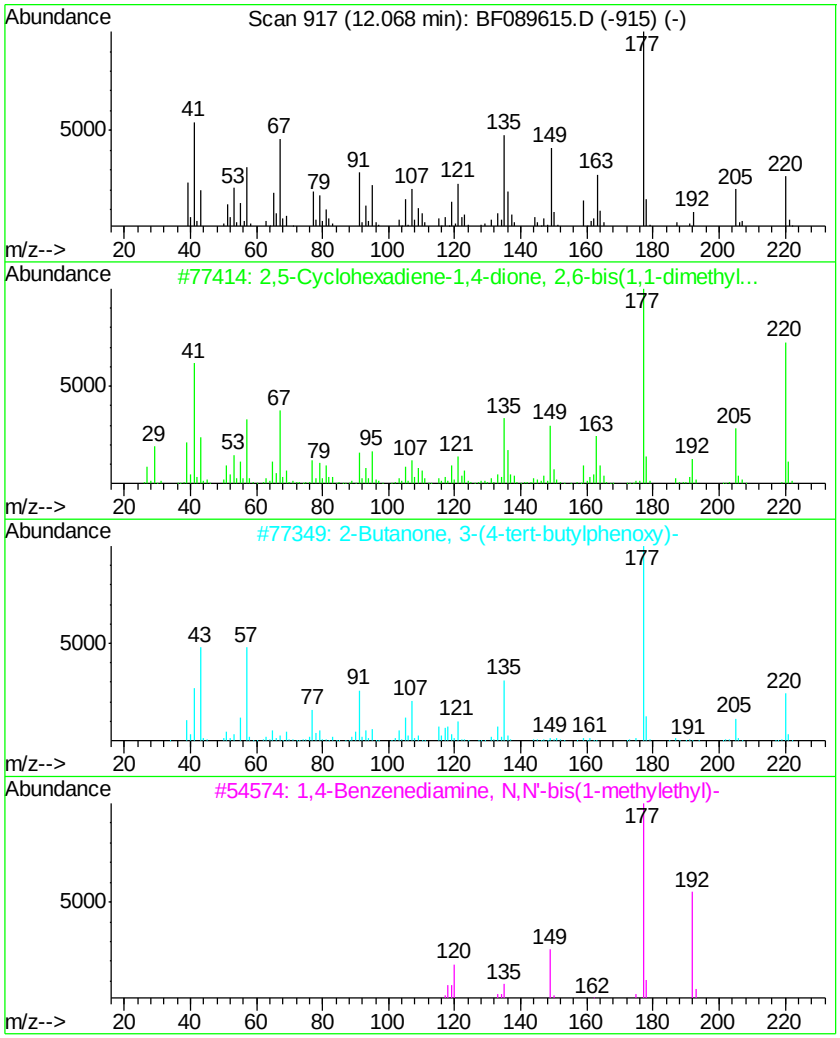
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

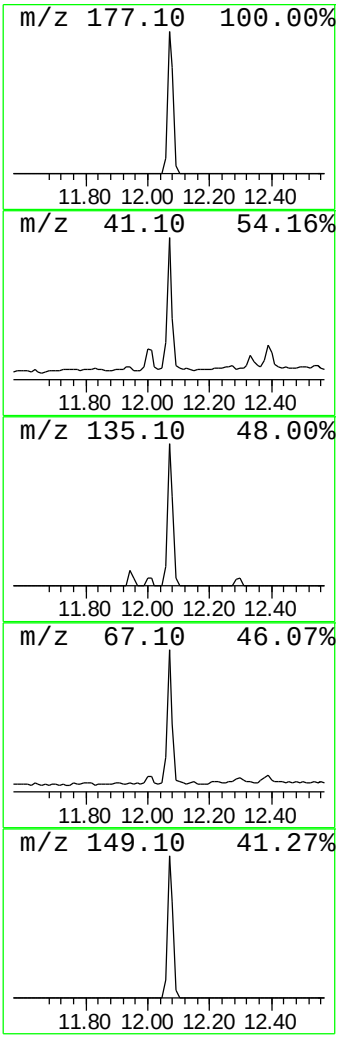
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	10.69 ng	212959	Acenaphthene-d10	12.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	46
3	1,4-Benzenediamine, N,N'-bis(1-m...	192	C12H20N2	004251-01-8	43
4	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	30
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	30





Library Search Compound Report

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ClientSampleId :
GW-65-10.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

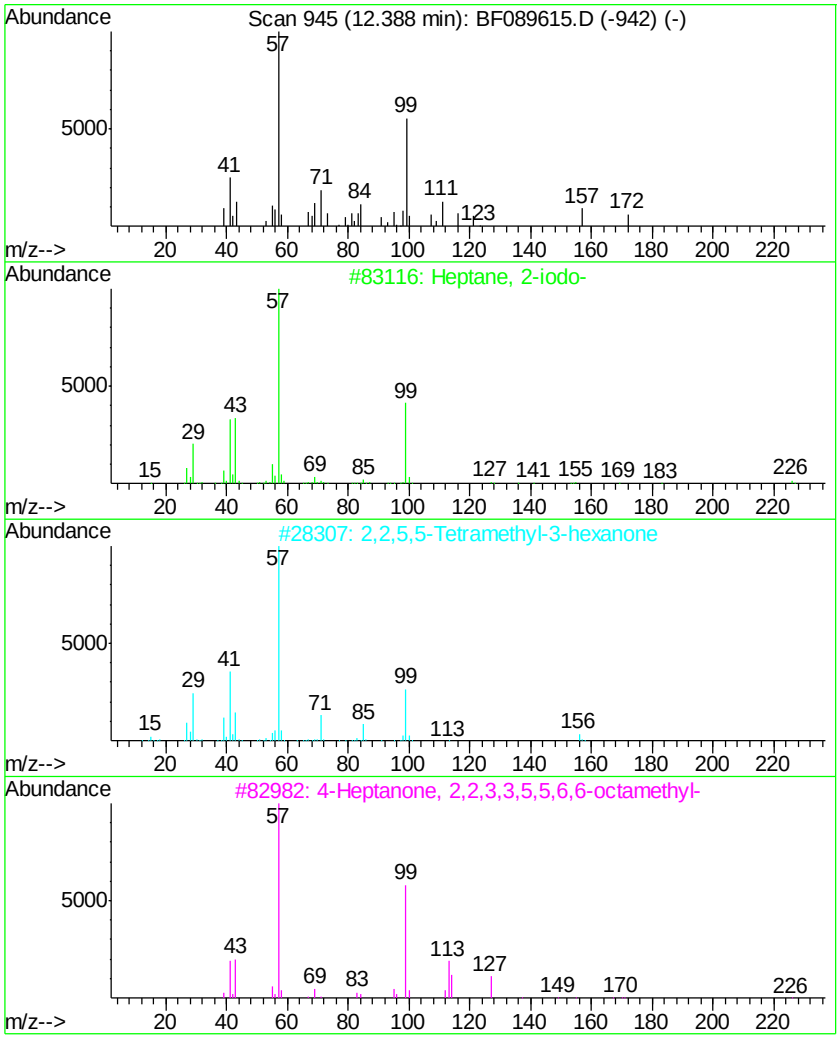
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

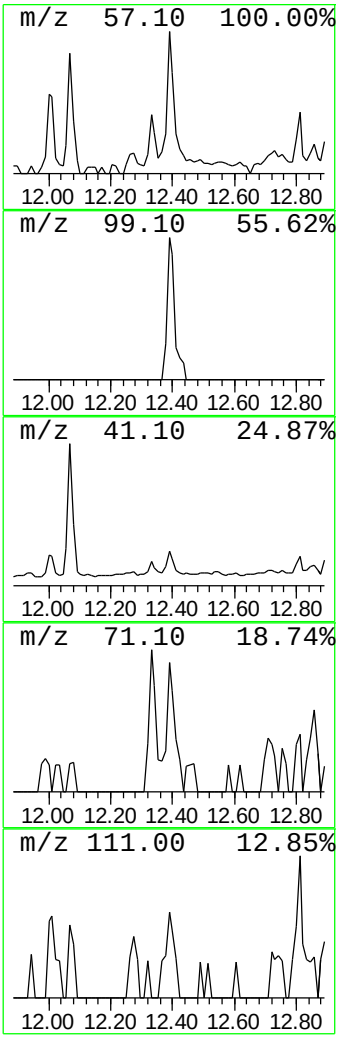
****

Peak Number 6 unknown12.39 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	2.59 ng	51566	Acenaphthene-d10	12.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-iodo-	226	C7H15I	018589-29-2	43
2	2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	43
3	4-Heptanone, 2,2,3,3,5,5,6,6-oct...	226	C15H30O	016424-66-1	37
4	Heptane, 3-bromo-	178	C7H15Br	001974-05-6	37
5	4-Heptanone, 5,5-diethyl-2,2,3,3...	226	C15H30O	016424-67-2	37





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Sample : H4288-21
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Instrument :
BNA_F
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GW-65-10.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

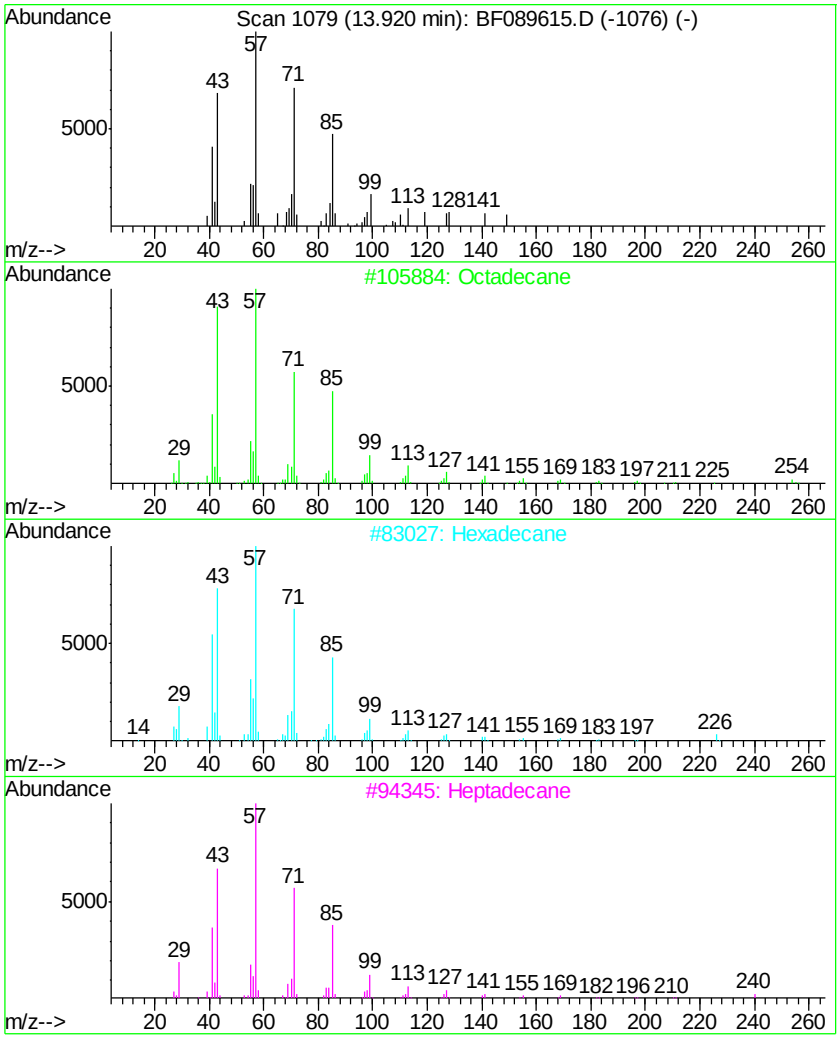
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

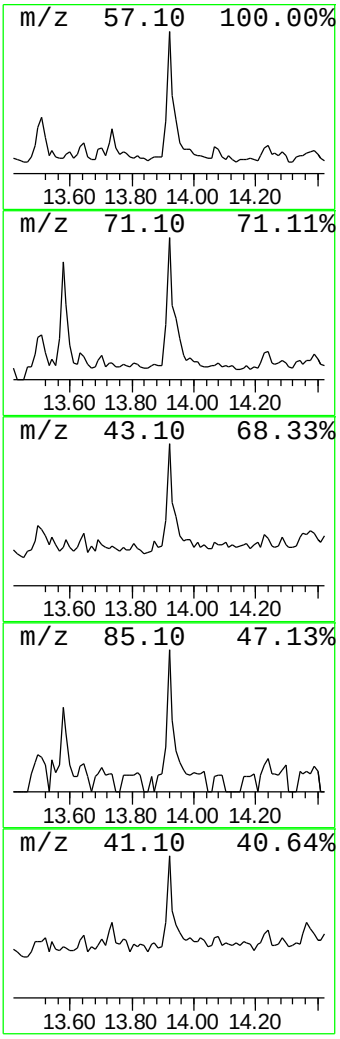
****

Peak Number 7 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	2.30 ng	46082	Phenanthrene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Heptadecane	240	C17H36	000629-78-7	72
4	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	64
5	Nonane	128	C9H20	000111-84-2	64





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

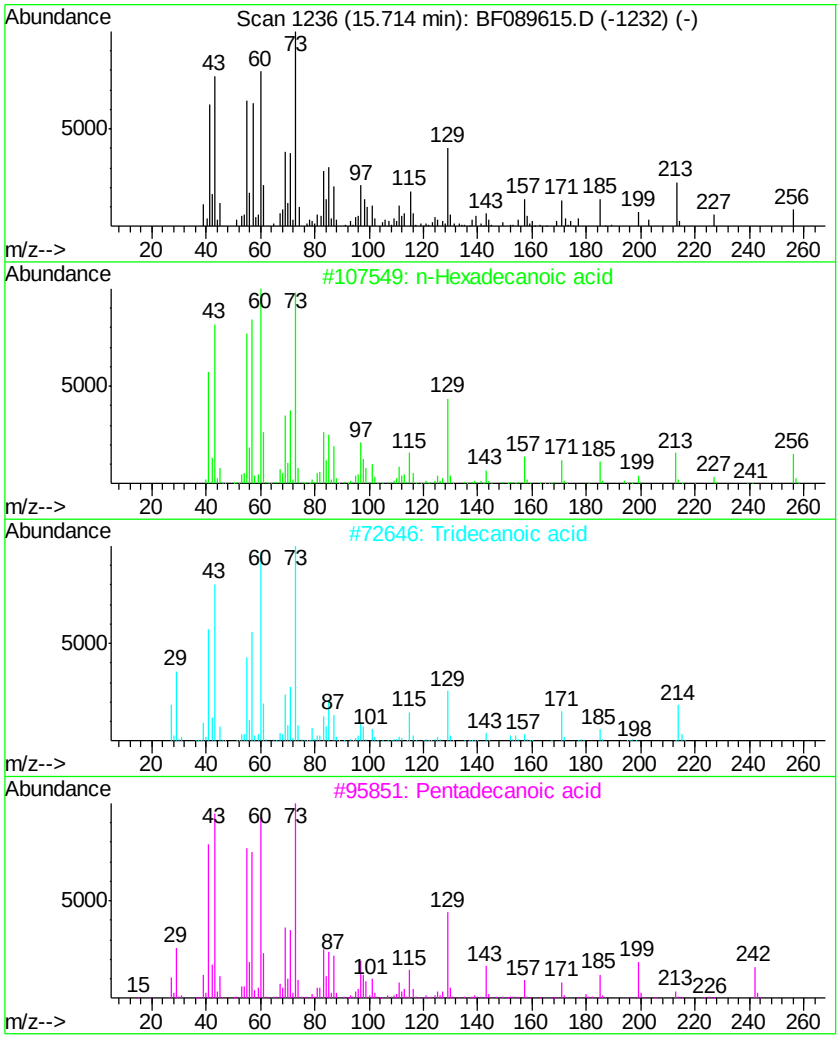
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

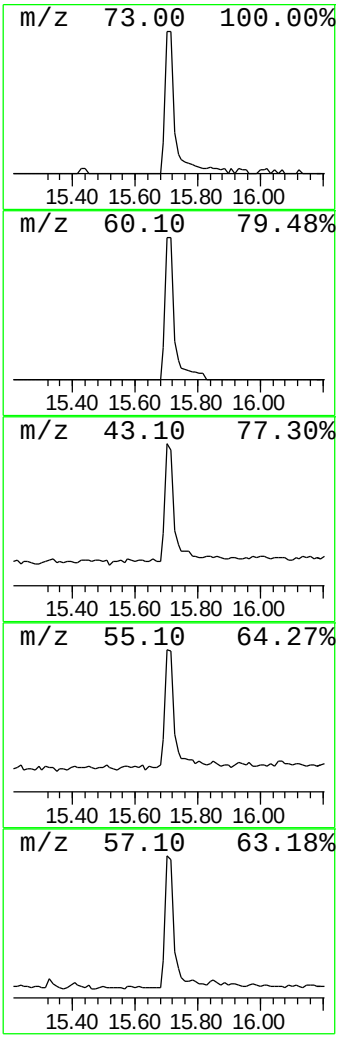
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	12.14 ng	243746	Phenanthrene-d10	14.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Operator : UM/SJ
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BNA_F
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GW-65-10.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

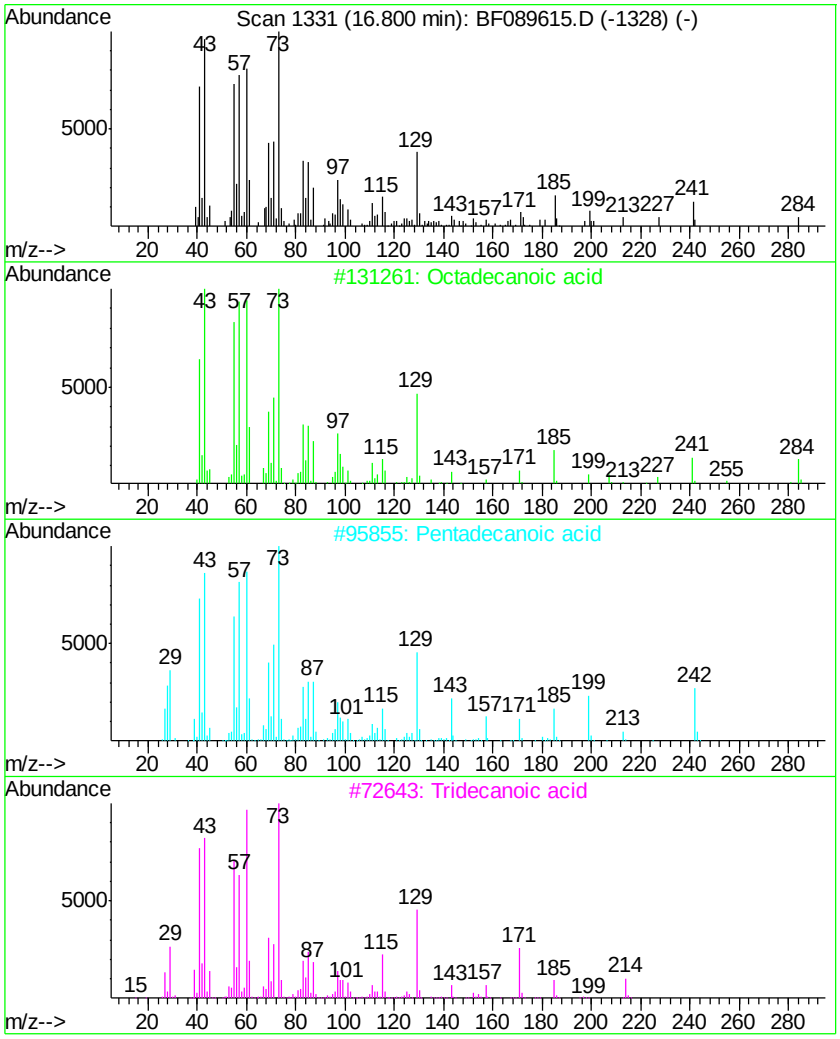
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

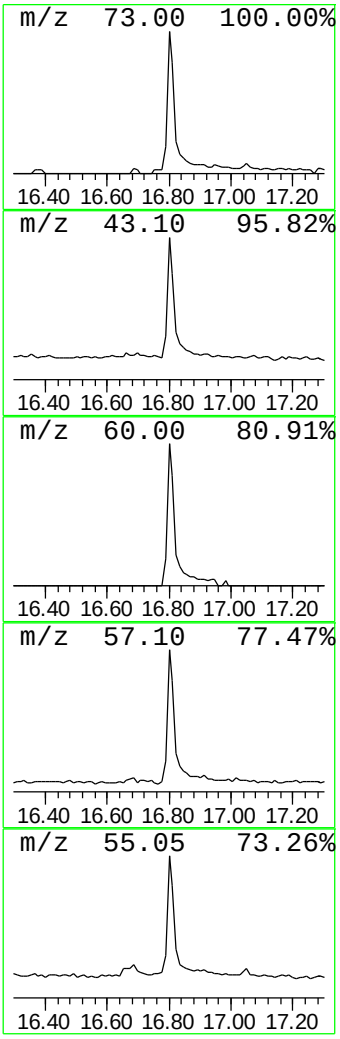
****

Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.80	18.95 ng	261975	Chrysene-d12	18.39

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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	49
5	Undecanoic acid	186	C11H22O2	000112-37-8	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080416\
Data File : BF089615.D
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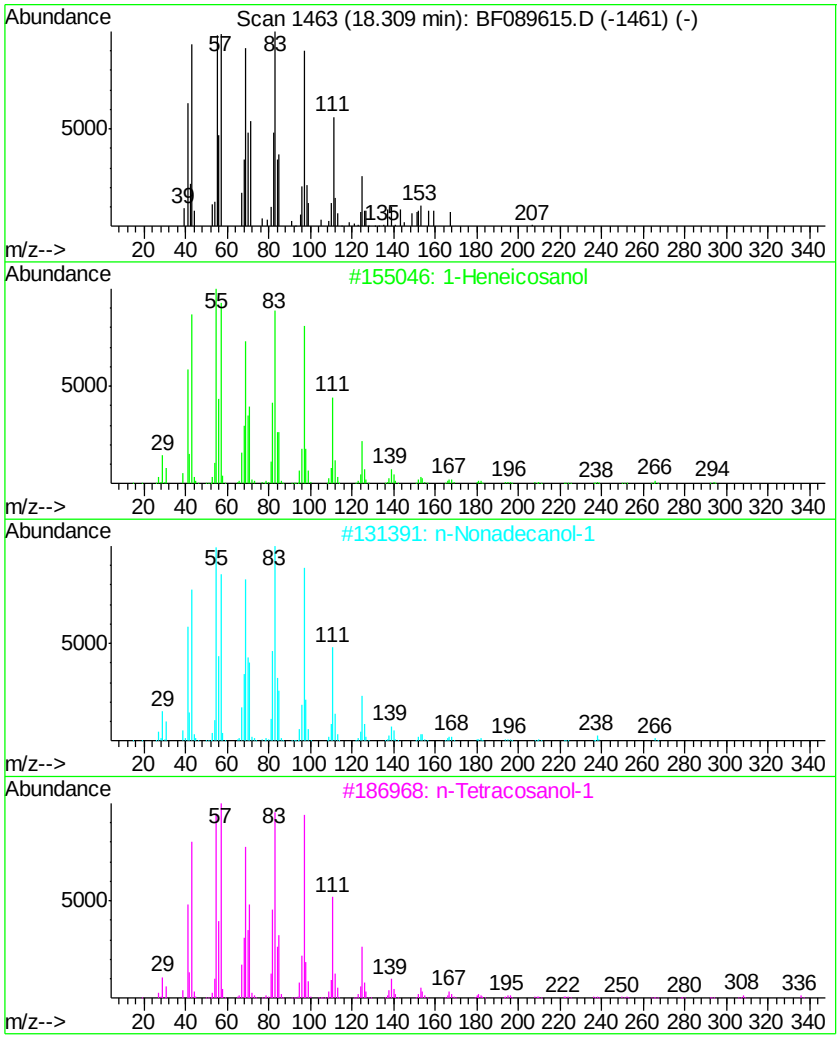
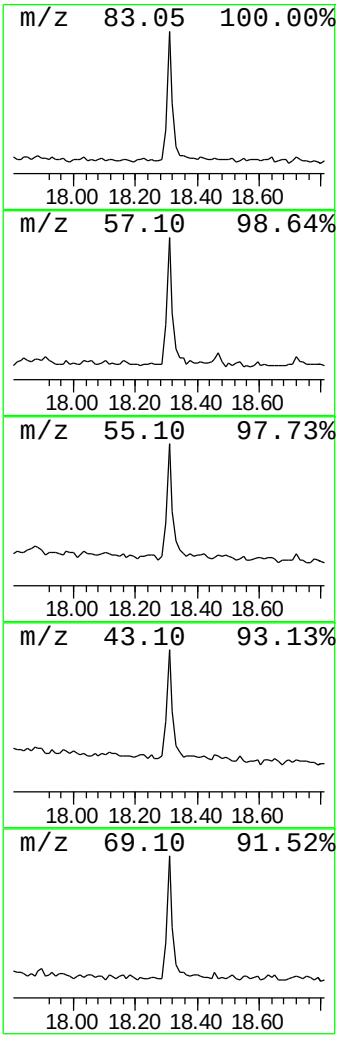
****

Peak Number 10 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	5.55 ng	76731	Chrysene-d12	18.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	1-Nonadecene	266	C19H38	018435-45-5	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080416\
Data File : BF089615.D
Acq On : 5 Aug 2016 6:23
Operator : UM/SJ
Sample : H4288-21
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-65-10.0-15.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	4.65	5.4	ng	60175	1	7.45	224406	20.0
unknown7.08	7.08	90.5	ng	1014850	1	7.45	224406	20.0
Phenol, 3-(1,1-di...	12.01	2.7	ng	54245	3	12.30	398598	20.0
2,5-Cyclohexadien...	12.07	10.7	ng	212959	3	12.30	398598	20.0
unknown12.39	12.39	2.6	ng	51566	3	12.30	398598	20.0
Octadecane	13.92	2.3	ng	46082	4	14.69	401535	20.0
n-Hexadecanoic acid	15.71	12.1	ng	243746	4	14.69	401535	20.0
Octadecanoic acid	16.80	18.9	ng	261975	5	18.39	276442	20.0
1-Heneicosanol	18.31	5.5	ng	76731	5	18.39	276442	20.0