LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

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-BF010918.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	4.922	478	482	489	rVB	143277	163504	3.27%	0.429%
2	5.334	547	552	555	rBV	3098959	2838657	56.78%	7.452%
3	6.357	722	726	733	rVB	1967610	1758405	35.17%	4.616%
4	6.498	745	750	753	rBV	4976915	4750980	95.03%	12.472%
5	6.728	785	789	793	rBV	1720916	1350184	27.01%	3.544%
6	6.792	797	800	805	rVB	106642	89046	1.78%	0.234%
7	6.886	811	816	819	rBV	4835875	4484451	89.70%	11.773%
8	7.298	874	886	889	rBV	3670796	3754227	75.09%	9.856%
9	7.451	908	912	914	rBV2	82796	78387	1.57%	0.206%
10	7.486	915	918	921	rVB	77556	63081	1.26%	0.166%
11	7.534	922	926	928	rBV2	64689	60010	1.20%	0.158%
12	7.692	946	953	956	rBV8	32291	69441	1.39%	0.182%
13	7.757	959	964	967	rVB4	52501	66355	1.33%	0.174%
14	7.986	998	1003	1004	rBV3	51451	68884	1.38%	0.181%
15	8.010	1004	1007	1010	rVB	1959016	1534118	30.69%	4.027%
16	8.381	1065	1070	1073	rBV5	70585	122146	2.44%	0.321%
17	8.569	1099	1102	1107	rVB2	93935	94469	1.89%	0.248%
18	8.822	1142	1145	1148	rBV	91040	75164	1.50%	0.197%
19	8.857	1148	1151	1156	rVB6	47164	65340	1.31%	0.172%
20	8.933	1161	1164	1170	rBV7	36403	80727	1.61%	0.212%
21	9.092	1185	1191	1194	rBV	5515344	4999456	100.00%	13.125%
22	9.210	1209	1211	1214	rVB	94271	73989	1.48%	0.194%
23	9.275	1220	1222	1229	rVB5	67401	89938	1.80%	0.236%
24	9.480	1255	1257	1260	rVB	89991	73783	1.48%	0.194%
25	9.680	1289	1291	1296	rVB2	105302	125947	2.52%	0.331%
26	9.727	1297	1299	1301	rVV2	62109	58225	1.16%	0.153%
27	9.763	1302	1305	1308	rVV2	1478098	1272576	25.45%	3.341%
28	9.792	1308	1310	1313	rVB	296008	255408	5.11%	0.670%
29	10.310	1395	1398	1402	rVB2	160489	134989	2.70%	0.354%
30	10.480	1424	1427	1430	rBV	125132	103364	2.07%	0.271%
31	10.551	1435	1439	1442	rBV	2317836	2188634	43.78%	5.746%
32	10.663	1456	1458	1462	rVB3	88103	77191	1.54%	0.203%
33	11.245	1554	1557	1560	rBV	1238038	1043812	20.88%	2.740%
34	11.322	1568	1570	1573	rVB	103632	75220	1.50%	0.197%

LSC Area Percent Report

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Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

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-BF010918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.792	1647	1650	1652	rBV	222013	195108	3.90%	0.512%
36	12.574	1781	1783	1787	rBV	207818	191288	3.83%	0.502%
37	12.727	1806	1809	1814	rVB	458896	445706	8.92%	1.170%
38	12.839	1824	1828	1831	rBV	3421484	3115765	62.32%	8.179%
39	13.733	1978	1980	1984	rVB2	270039	229933	4.60%	0.604%
40	13.886	2002	2006	2009	rBV	1146927	1048997	20.98%	2.754%
41	15.304	2243	2247	2251	rVB2	622429	725465	14.51%	1.904%

Sum of corrected areas: 38092370

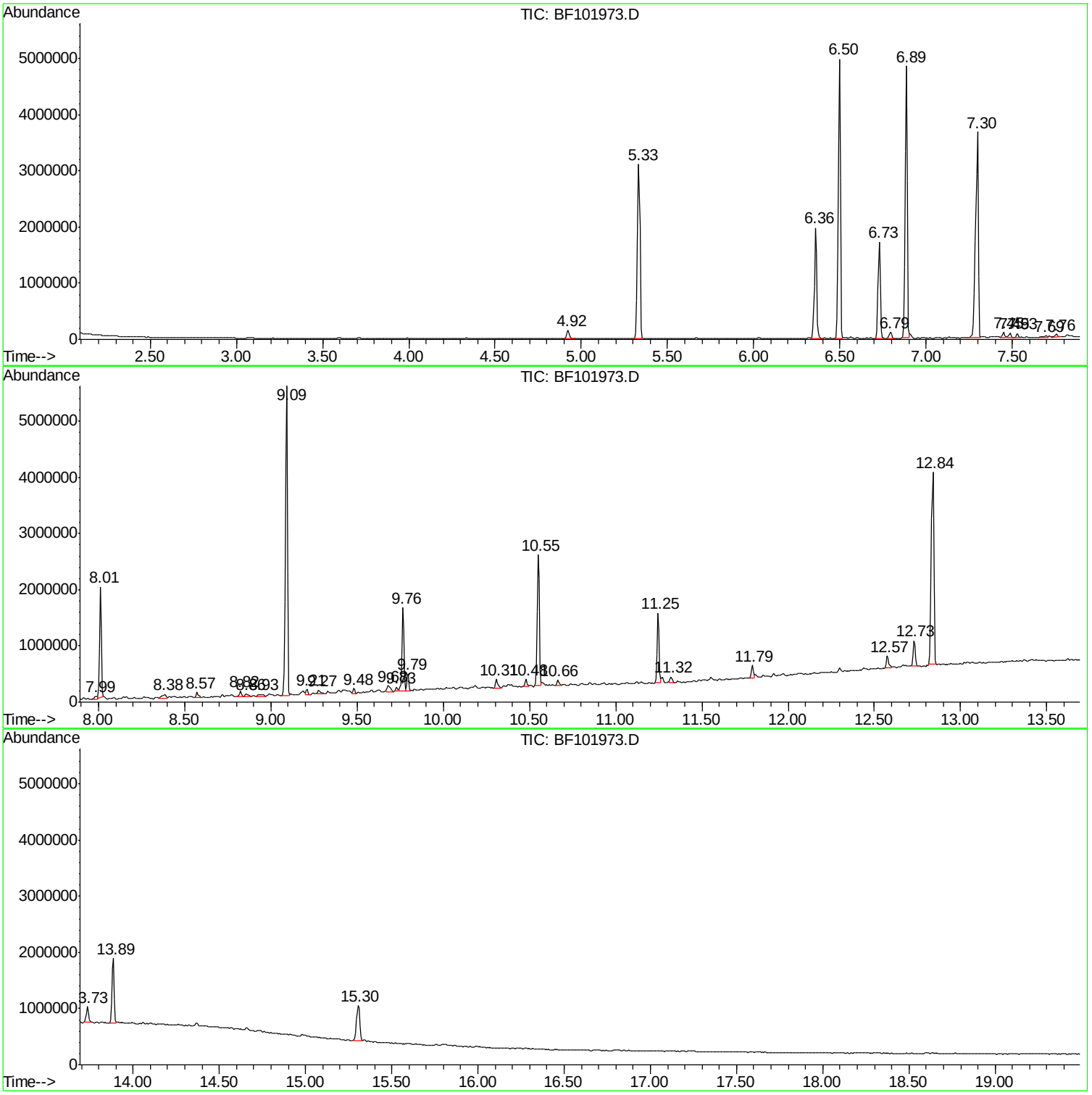
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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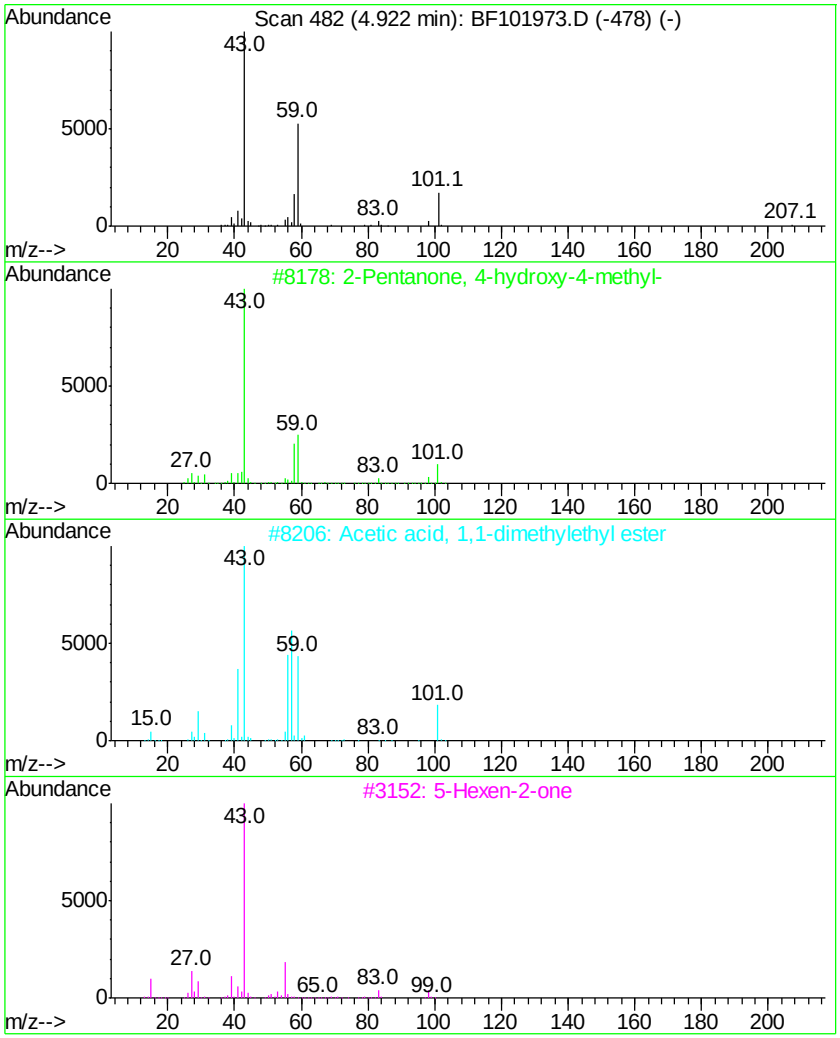
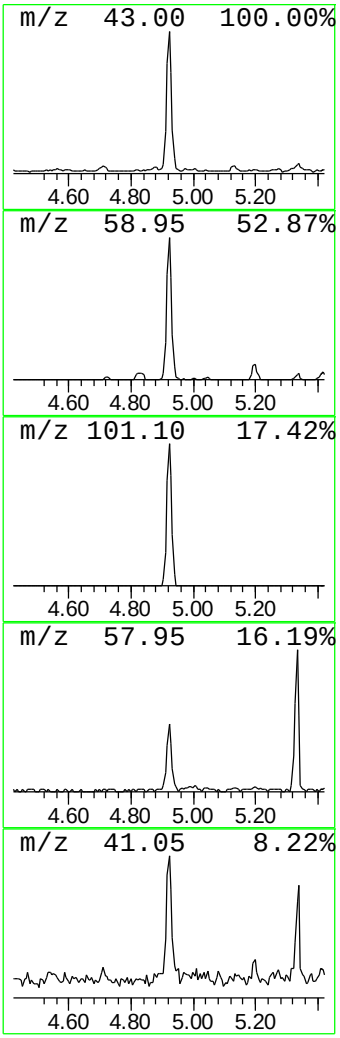
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.42 ng	163504	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

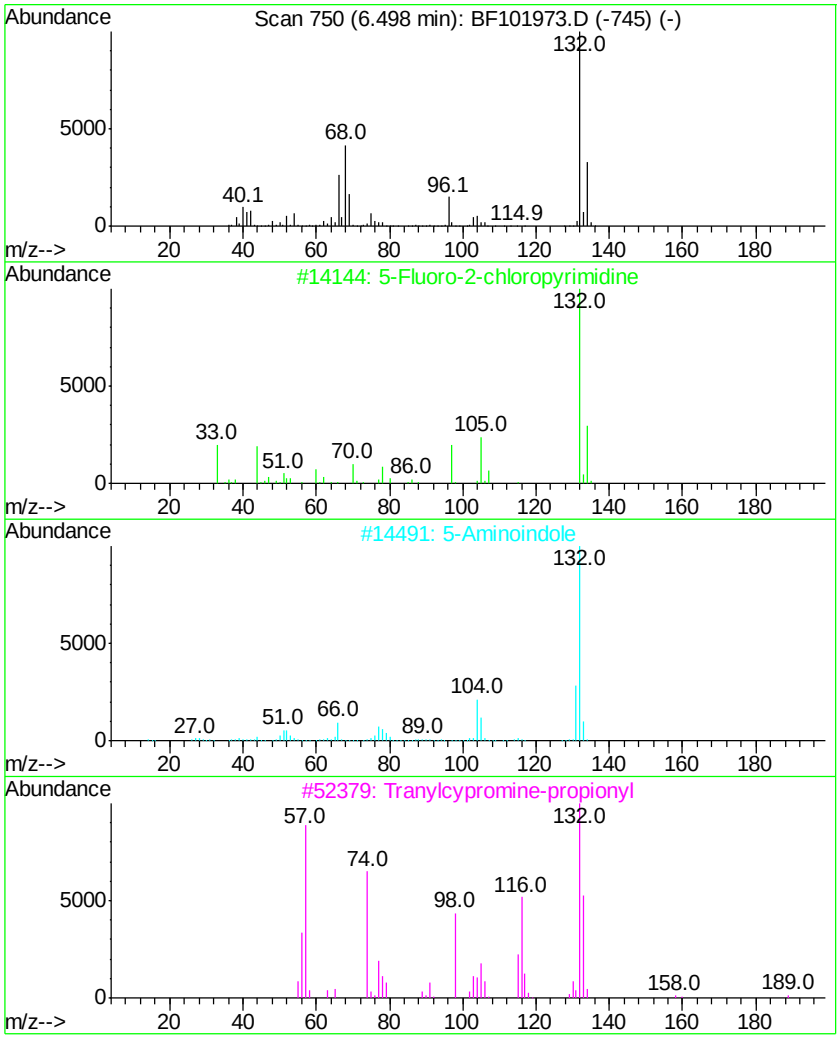
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

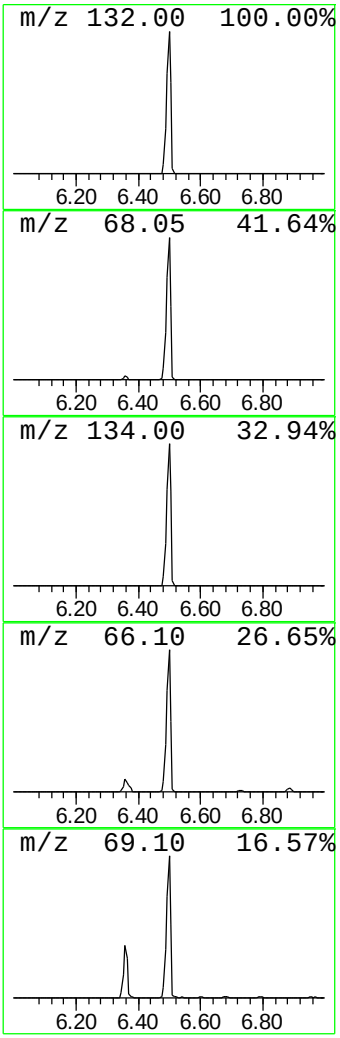
****

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	70.38 ng	4750980	1,4-Dichlorobenzene-d4	6.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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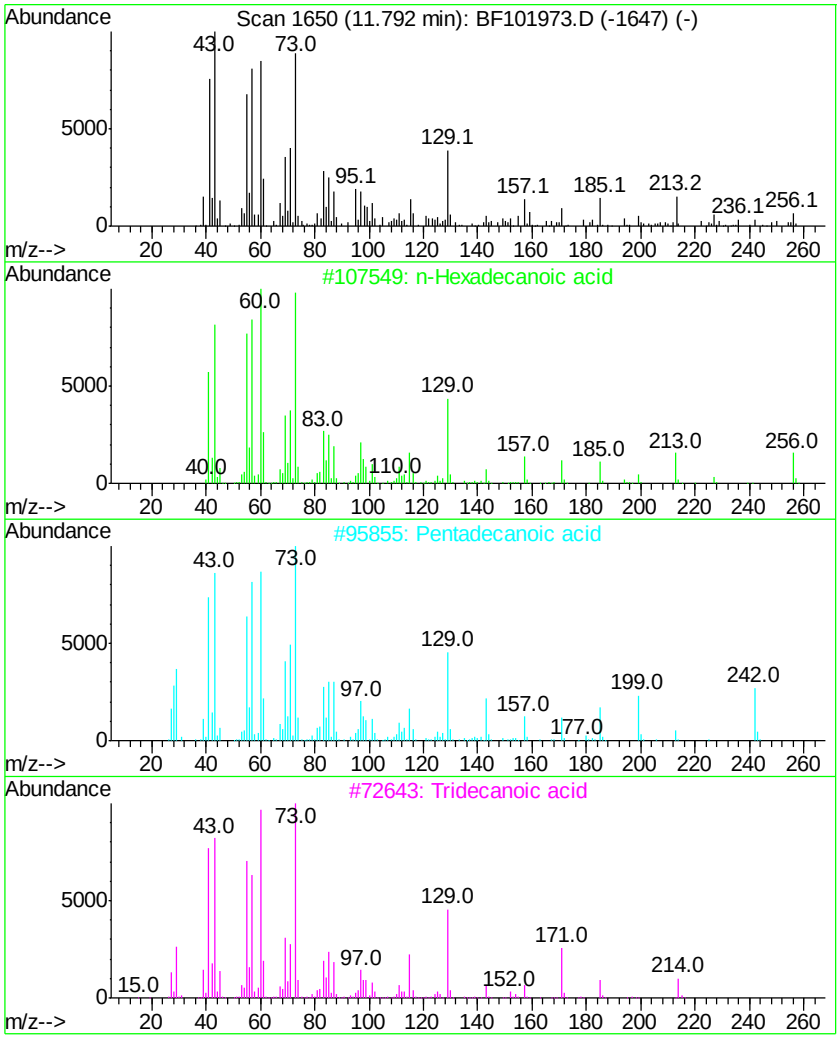
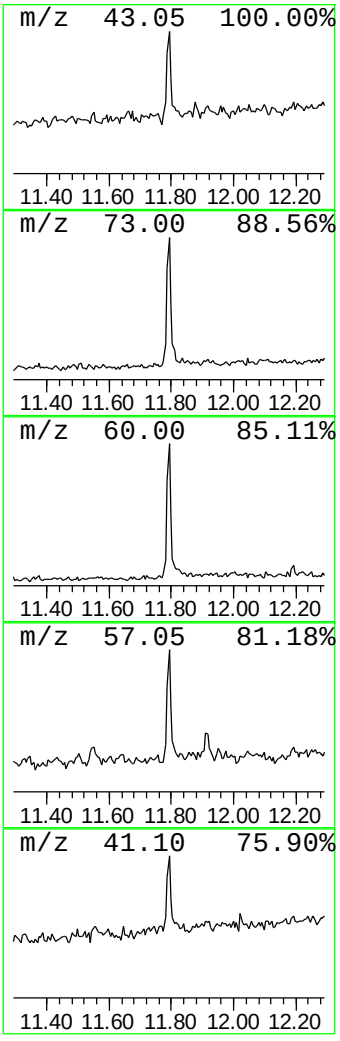
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	3.74 ng	195108	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Octanoic acid	144	C8H16O2	000124-07-2	30
5	Pentadecane	212	C15H32	000629-62-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF010918\
Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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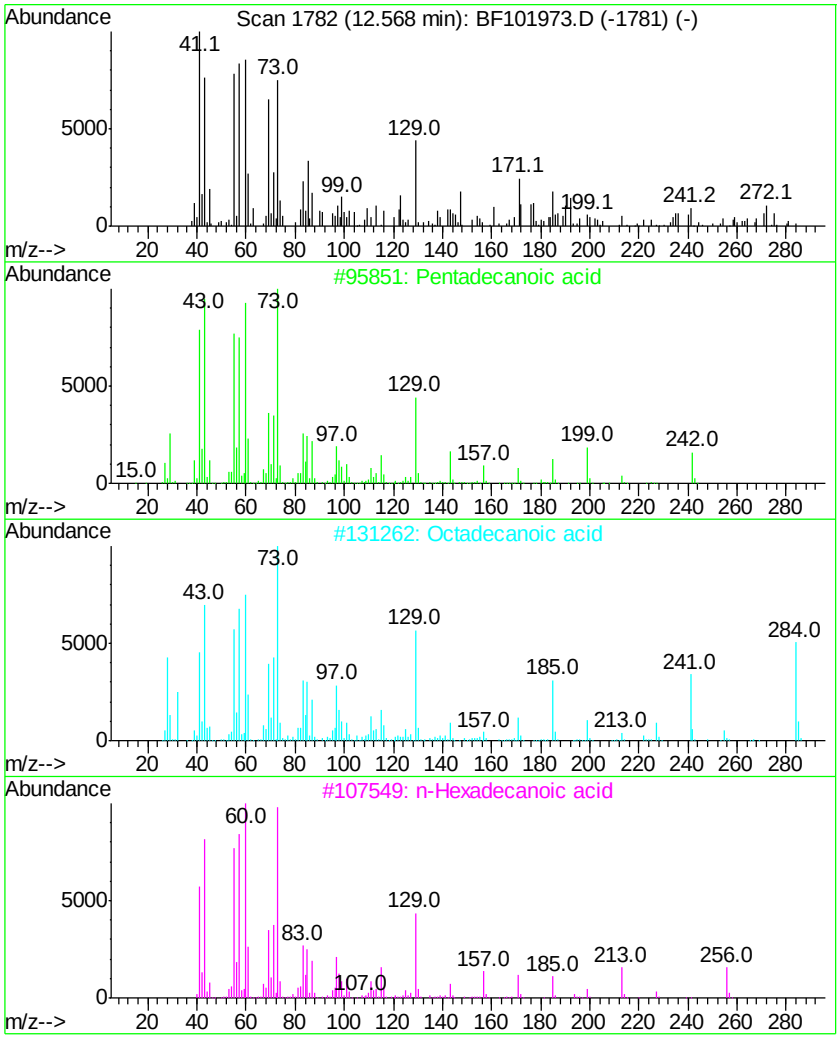
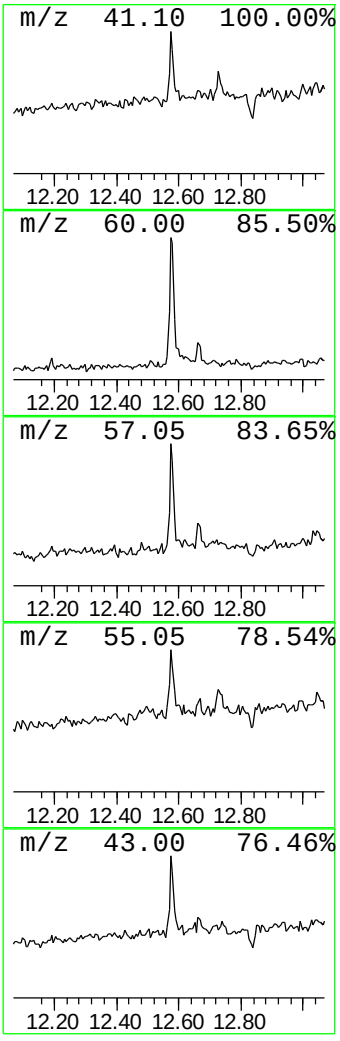
Peak Number 6 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.65 ng	191288	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	Octadecanoic acid	284	C18H36O2	000057-11-4	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64





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Operator : SJ/JU
Sample : J1049-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

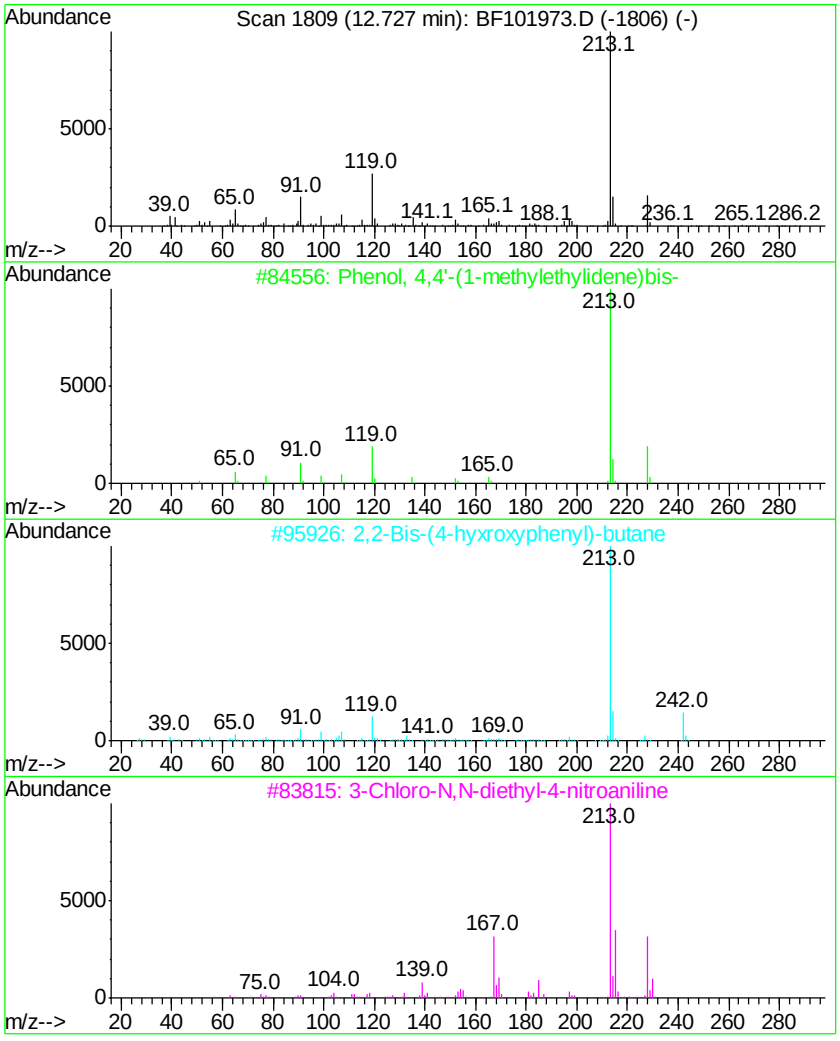
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

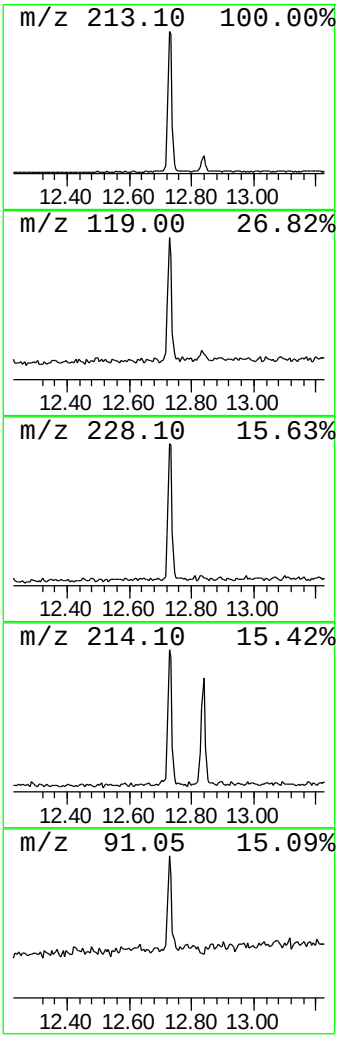
****

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	8.50 ng	445706	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
3	3-Chloro-N,N-diethyl-4-nitroaniline	228	C10H13ClN2O2	1000110-36-0	42
4	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	40
5	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	40





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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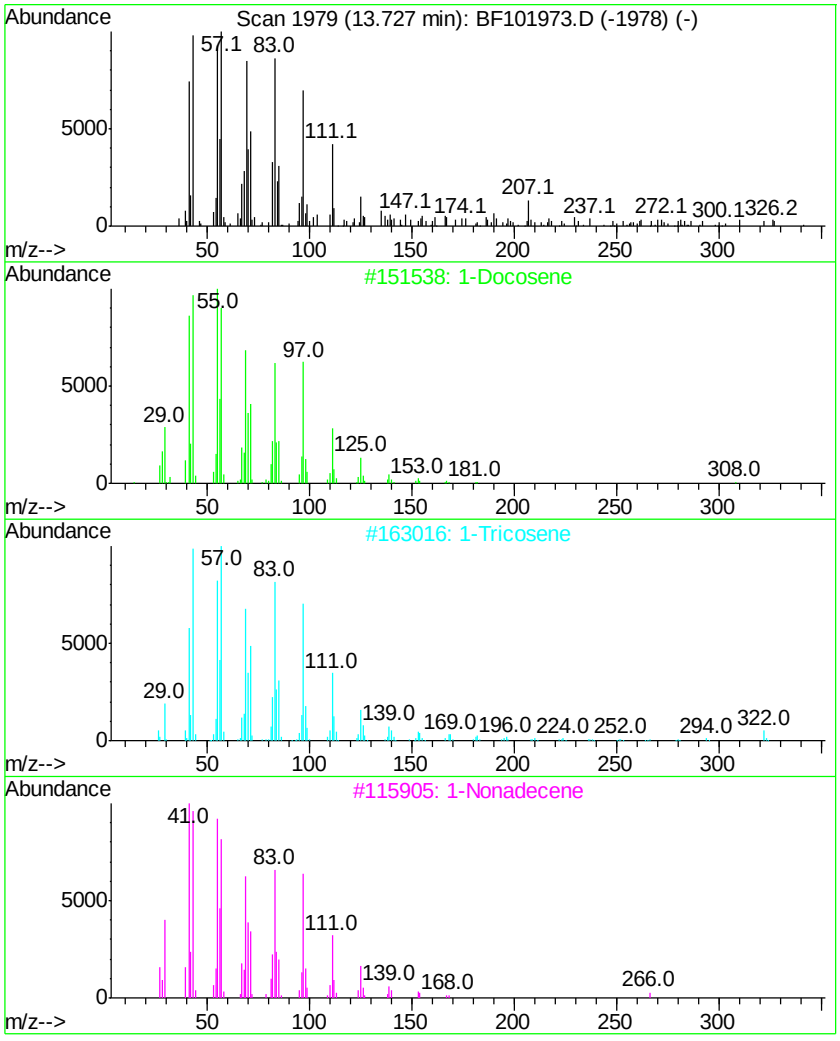
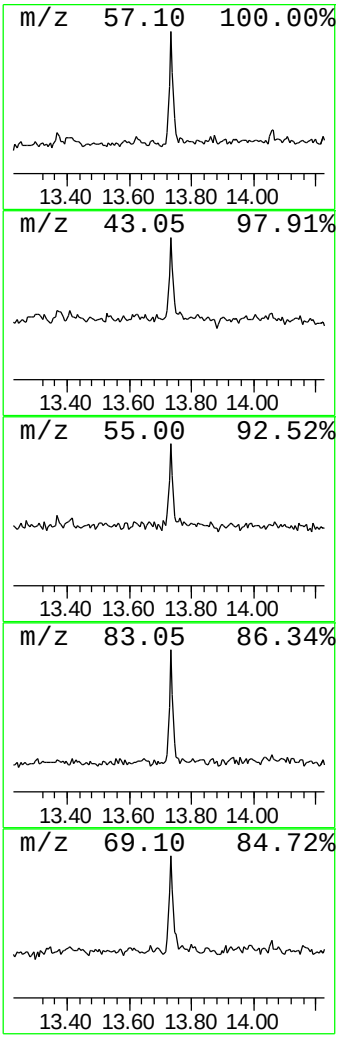
Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.38 ng	229933	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Tricosene	322	C23H46	018835-32-0	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010918\
Data File : BF101973.D
Acq On : 10 Jan 2018 00:38
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	2.4	ng	163504	1	6.73	1350180	20.0
unknown6.50	6.50	70.4	ng	4750980	1	6.73	1350180	20.0
n-Hexadecanoic acid	11.79	3.7	ng	195108	4	11.25	1043810	20.0
Pentadecanoic acid	12.57	3.6	ng	191288	5	13.89	1049000	20.0
Phenol, 4,4'-(1-m...	12.73	8.5	ng	445706	5	13.89	1049000	20.0
1-Docosene	13.73	4.4	ng	229933	5	13.89	1049000	20.0