LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101504.D
Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121217-TIDO-E-D-S

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-BF121417.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	5.022	496	499	516	rVB	79781	111478	3.61%	0.523%
2	5.434	566	569	592	rBV	929569	1230104	39.88%	5.772%
3	6.457	739	743	761	rBV2	608705	866396	28.09%	4.065%
4	6.581	761	764	771	rBV	1920971	1929808	62.56%	9.055%
5	6.810	799	803	810	rBV	630368	559408	18.14%	2.625%
6	6.963	825	829	840	rBV	2638779	2617722	84.87%	12.283%
7	7.381	895	900	917	rBV	2017906	2043394	66.25%	9.588%
8	7.828	972	976	979	rBV2	25761	31790	1.03%	0.149%
9	7.928	989	993	1000	rVB	76126	65969	2.14%	0.310%
10	8.092	1017	1021	1024	rBV	716642	670883	21.75%	3.148%
11	8.804	1140	1142	1147	rBV	101673	95673	3.10%	0.449%
12	8.904	1153	1159	1167	rVB	82931	81218	2.63%	0.381%
13	9.169	1199	1204	1207	rBV	3095173	3084538	100.00%	14.473%
14	9.269	1217	1221	1225	rVB	53008	48382	1.57%	0.227%
15	9.563	1268	1271	1276	rVB	76483	68020	2.21%	0.319%
16	9.828	1313	1316	1317	rBV	48212	40778	1.32%	0.191%
17	9.845	1317	1319	1322	rVV2	637658	549017	17.80%	2.576%
18	9.881	1322	1325	1330	rVB	204916	179652	5.82%	0.843%
19	10.057	1351	1355	1359	rBV	109643	102110	3.31%	0.479%
20	10.398	1410	1413	1419	rBV	134597	117351	3.80%	0.551%
21	10.557	1437	1440	1443	rBV	43237	42610	1.38%	0.200%
22	10.645	1451	1455	1467	rBV	1010088	1082928	35.11%	5.081%
23	11.339	1569	1573	1575	rBV	579489	515907	16.73%	2.421%
24	11.363	1575	1577	1581	rVB	310117	257689	8.35%	1.209%
25	11.416	1584	1586	1591	rVV	30434	38703	1.25%	0.182%
26	11.857	1656	1661	1669	rBV2	299445	405763	13.15%	1.904%
27	12.563	1776	1781	1789	rBV2	250232	414113	13.43%	1.943%
28	12.639	1792	1794	1798	rVV4	62231	65068	2.11%	0.305%
29	12.792	1818	1820	1825	rVB2	89624	98500	3.19%	0.462%
30	12.922	1838	1842	1845	rBV	2512966	2450833	79.46%	11.500%
31	12.969	1845	1850	1856	rVB2	78082	136519	4.43%	0.641%
32	13.727	1977	1979	1982	rBV3	77268	96667	3.13%	0.454%
33	13.992	2020	2024	2030	rVB	615738	663902	21.52%	3.115%
34	15.463	2270	2274	2278	rBV	400105	549429	17.81%	2.578%

LSC Area Percent Report

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Data File : BF101504.D
Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
121217-TIDO-E-D-S

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

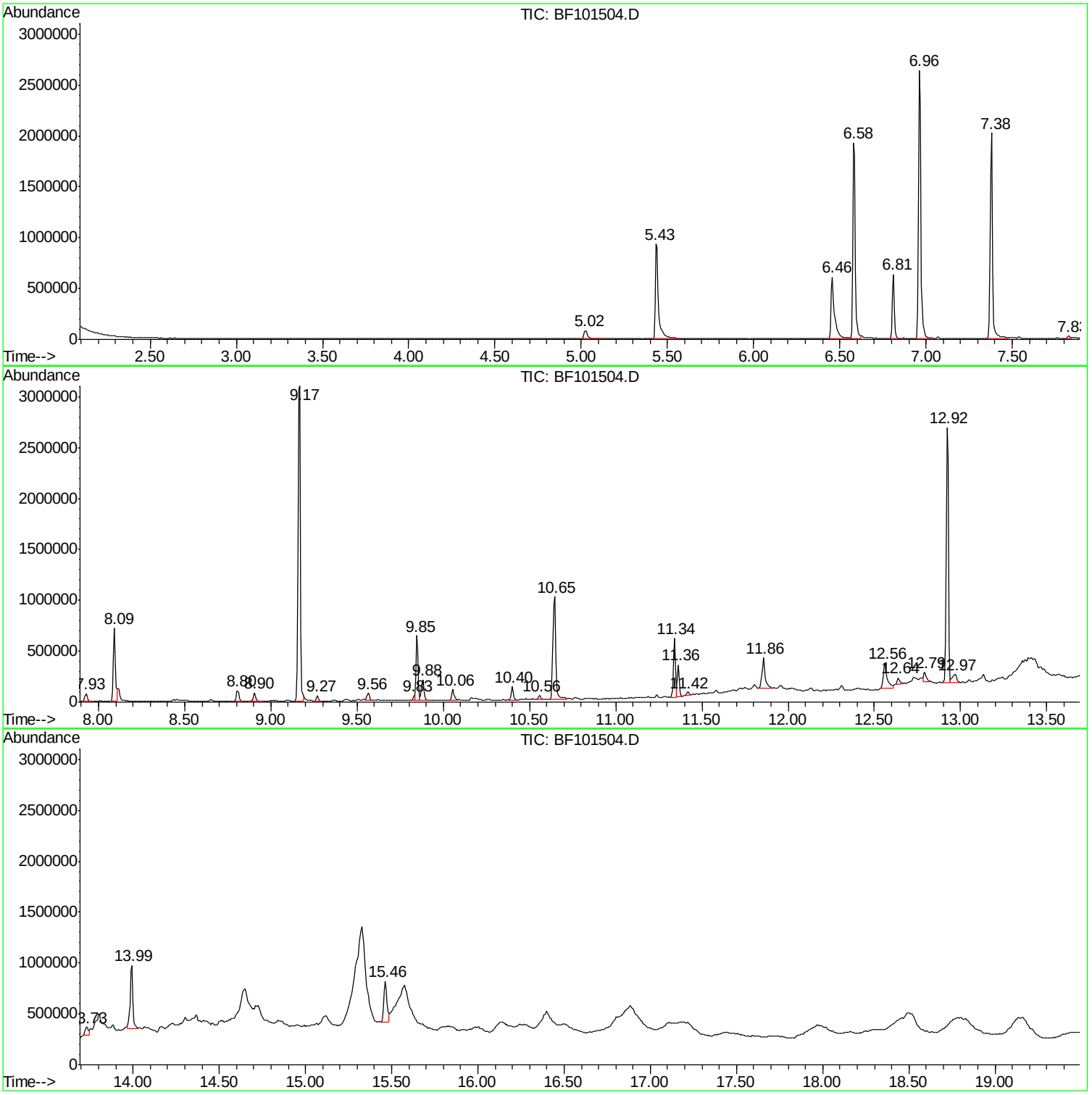
Sum of corrected areas: 21312322

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101504.D
Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF121817\
Data File : BF101504.D
Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

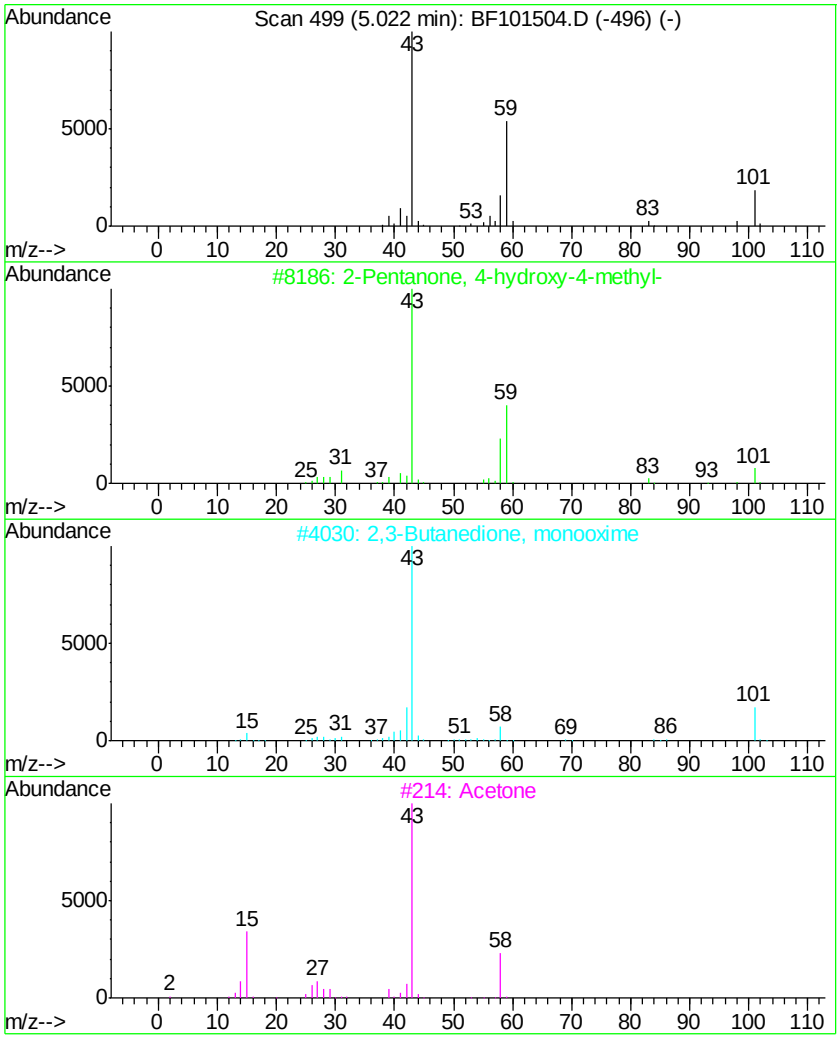
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

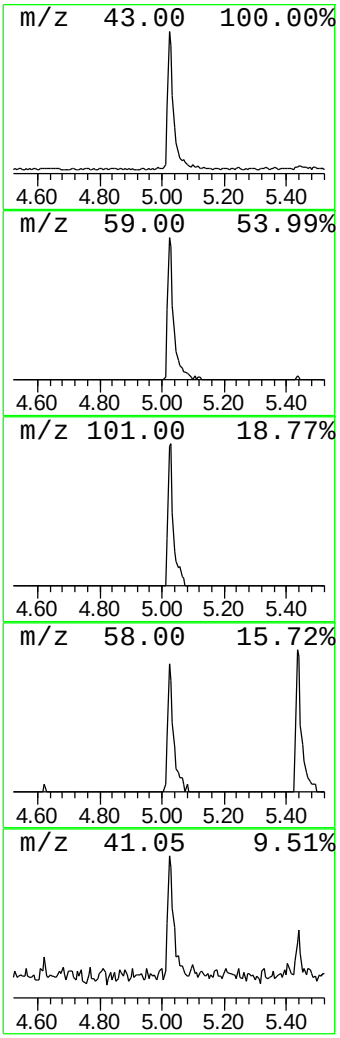
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.99 ng	111478	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Acetone	58	C3H6O	000067-64-1	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101504.D
Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

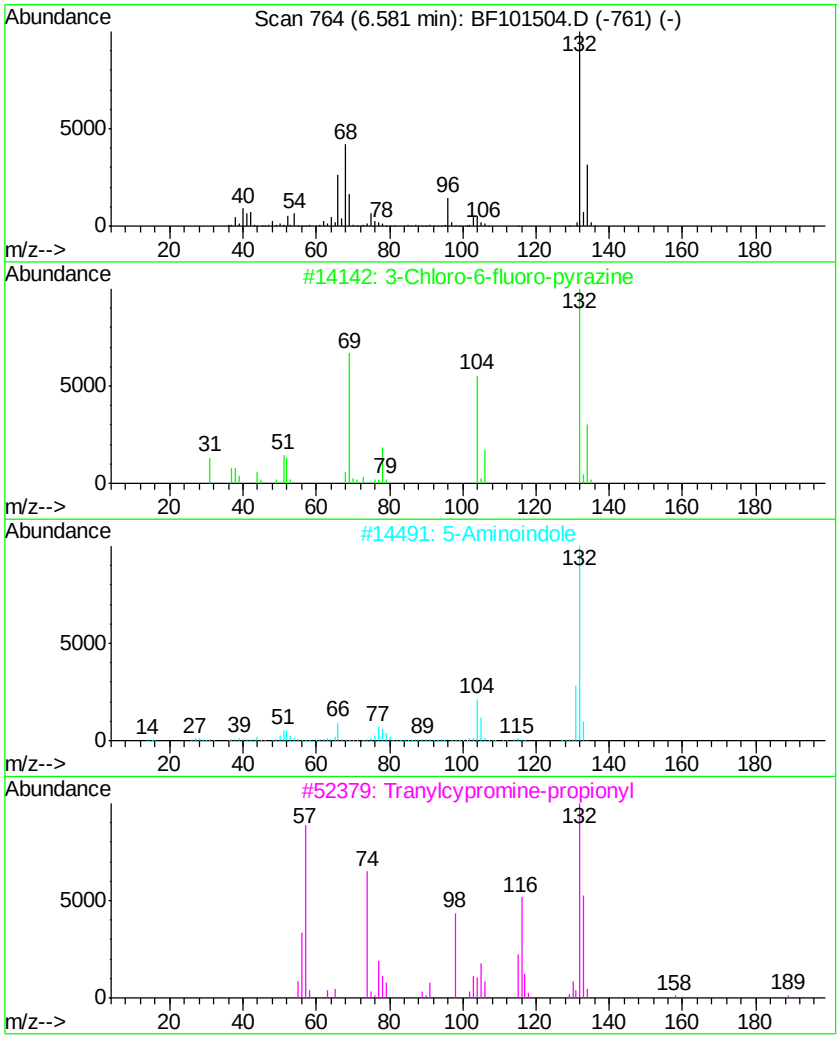
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

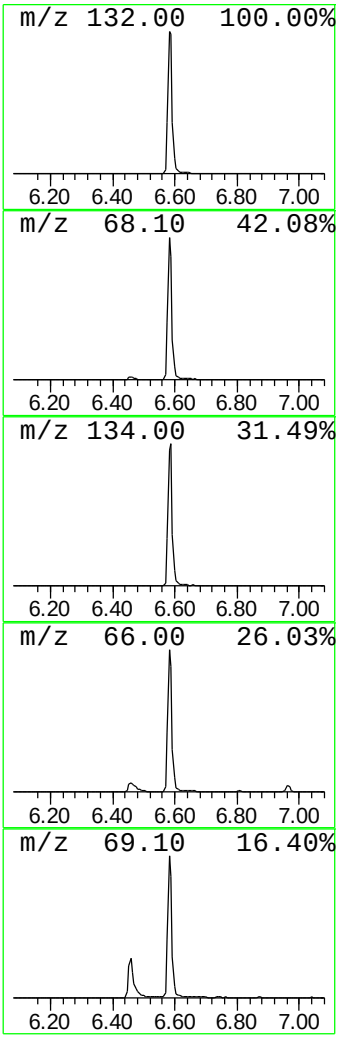
****

Peak Number 2 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	68.99 ng	1929810	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101504.D
Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

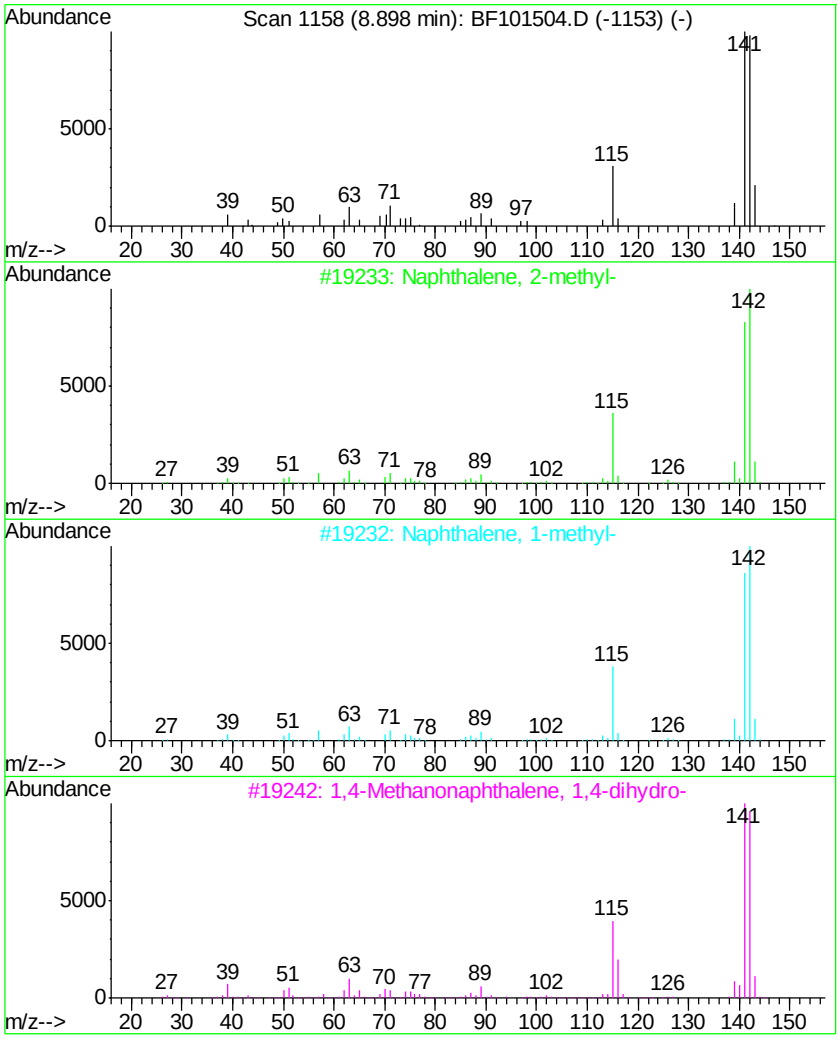
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

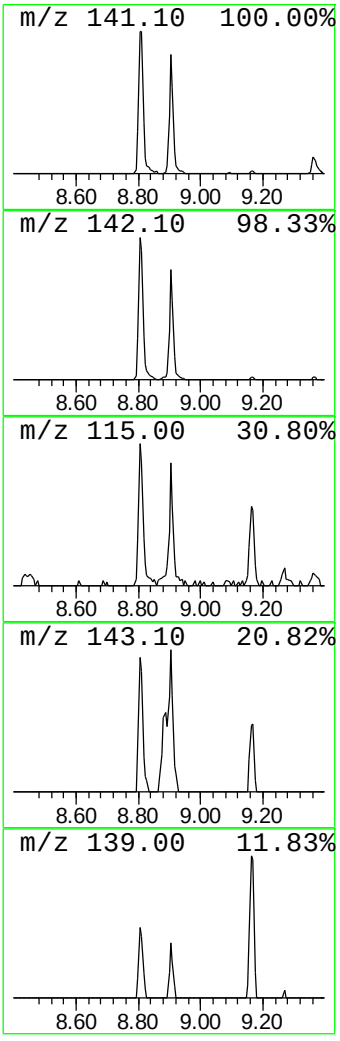
****

Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	2.42 ng	81218	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
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Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

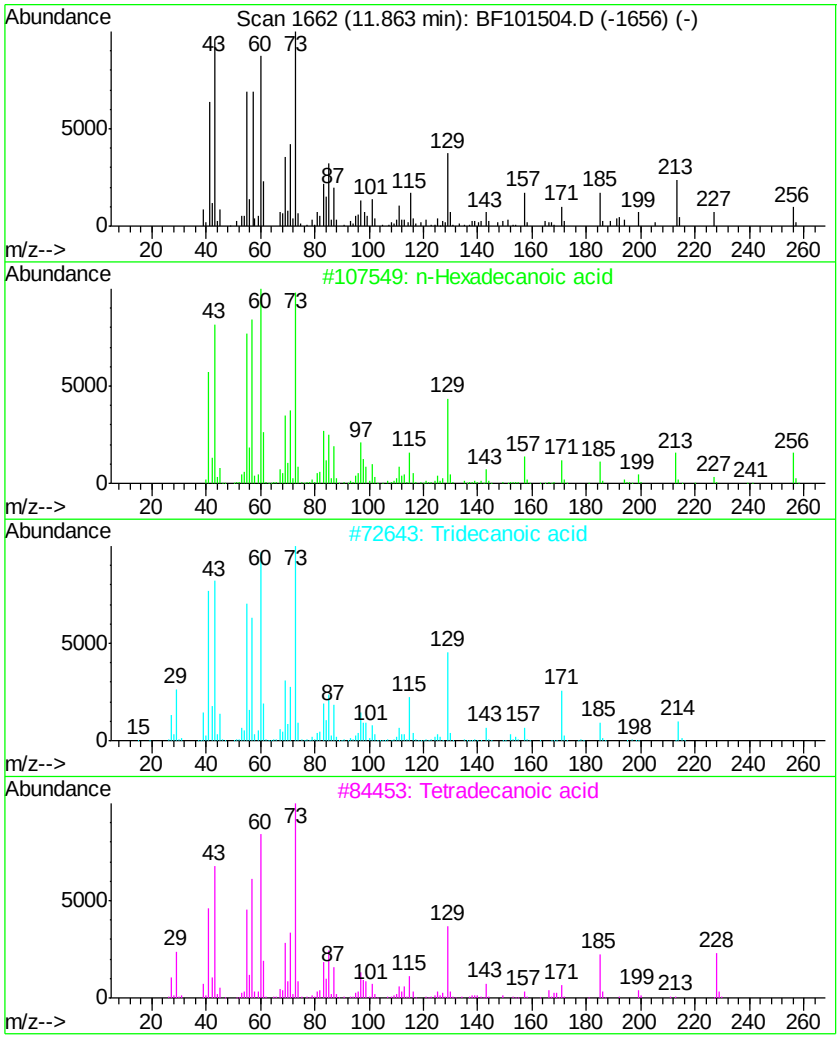
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

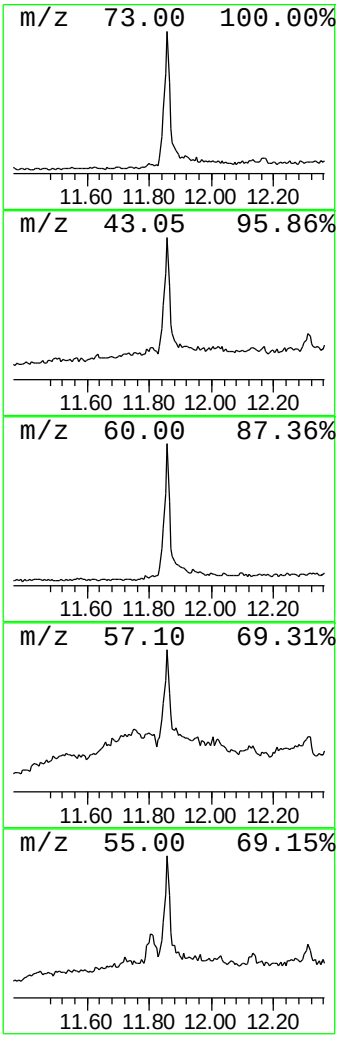
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	15.73 ng	405763	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
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Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

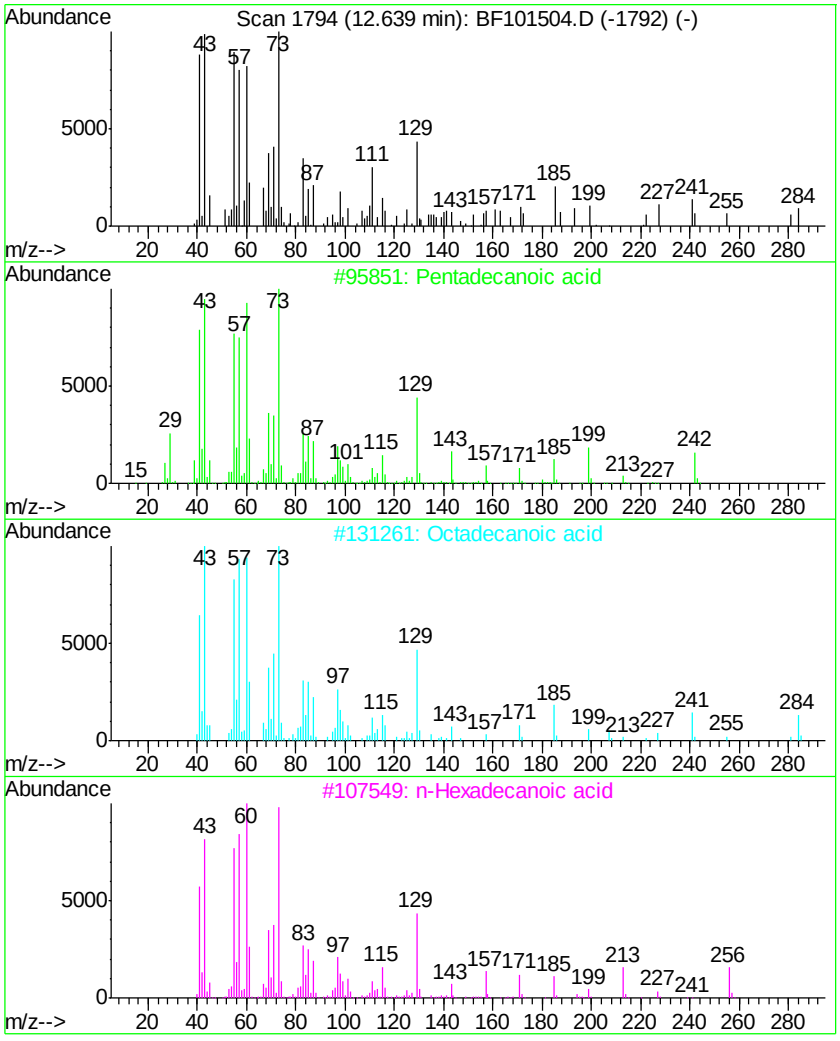
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

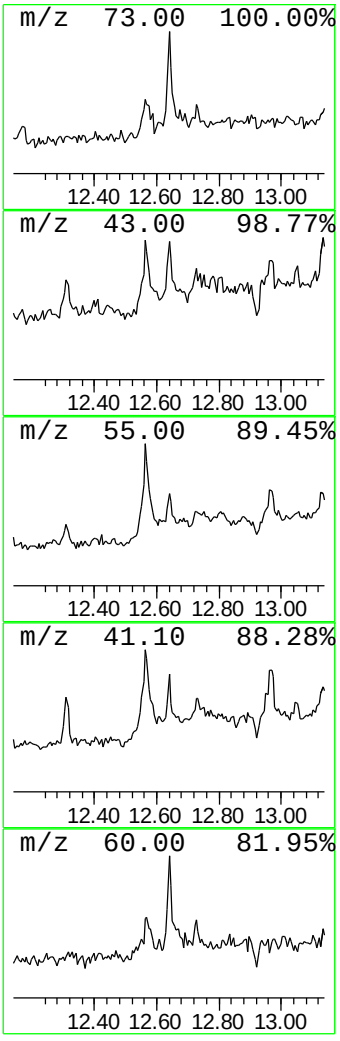
****

Peak Number 6 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.52 ng	65068	Phenanthrene-d10	11.34

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	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Data File : BF101504.D
Acq On : 19 Dec 2017 3:23
Operator : SJ/JU
Sample : I6909-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

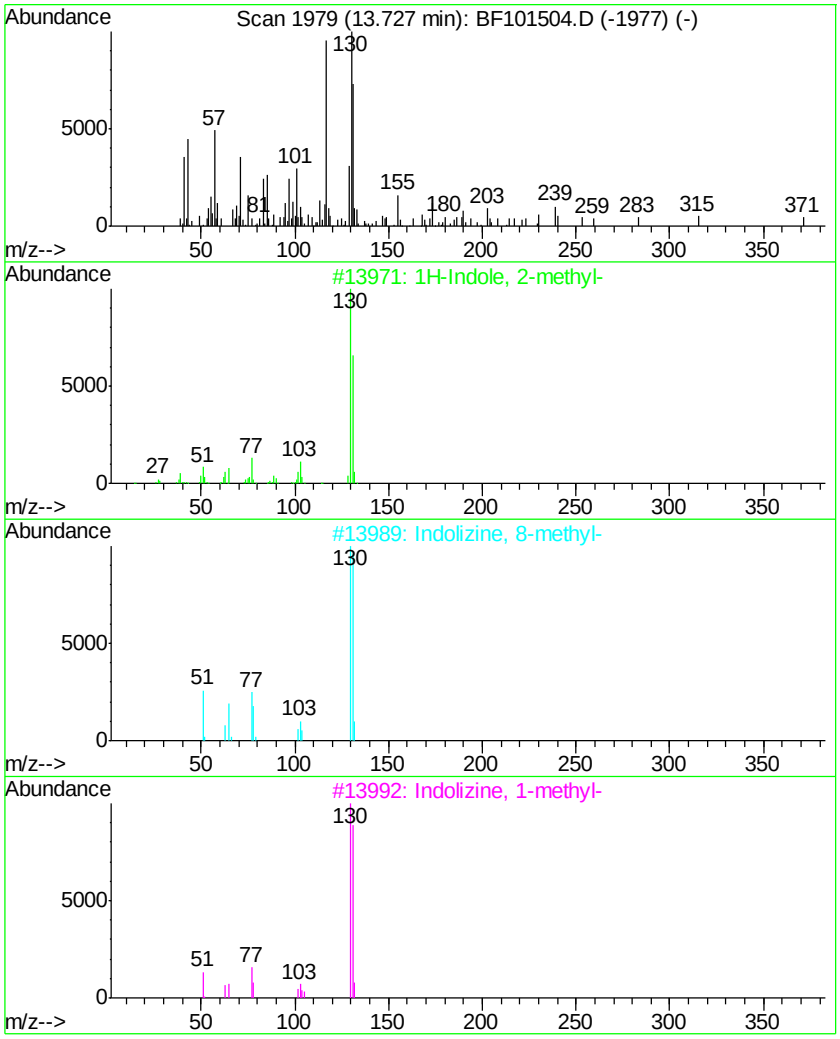
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

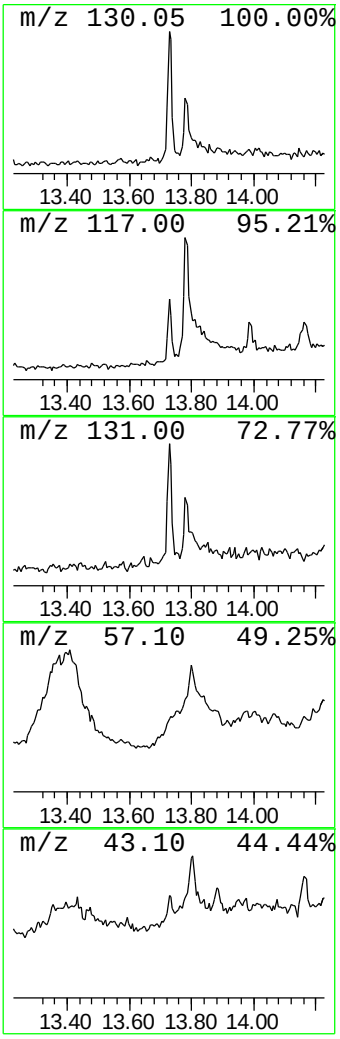
****

Peak Number 7 unknown13.73 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	2.91 ng	96667	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-	131	C9H9N	000095-20-5	30
2	Indolizine, 8-methyl-	131	C9H9N	031108-58-4	30
3	Indolizine, 1-methyl-	131	C9H9N	000767-61-3	30
4	1-Naphthalenol, 1,2,3,4-tetrahyd...	190	C12H14O2	021503-12-8	30
5	1H-Indole, 3-methyl-	131	C9H9N	000083-34-1	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101504.D
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Misc :
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Instrument : BNA_F
ClientSampleId : 121217-TIDO-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.02	4.0	ng	111478	1	6.81	559408	20.0
unknown6.58	6.58	69.0	ng	1929810	1	6.81	559408	20.0
Naphthalene, 2-me...	8.90	2.4	ng	81218	2	8.09	670883	20.0
n-Hexadecanoic acid	11.86	15.7	ng	405763	4	11.34	515907	20.0
Pentadecanoic acid	12.64	2.5	ng	65068	4	11.34	515907	20.0
unknown13.73	13.73	2.9	ng	96667	5	13.99	663902	20.0