LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102596.D
Acq On : 29 Jan 2018 14:36
Operator : SJ/JU
Sample : J1253-19 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-10(0-5)

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-BF012218.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	4.898	474	478	490	rBV	35294	47148	2.72%	0.242%
2	5.281	540	543	547	rBV	26214	39012	2.25%	0.201%
3	5.328	547	551	571	rVB	1563436	1694199	97.58%	8.709%
4	6.145	685	690	698	rBV7	18101	38946	2.24%	0.200%
5	6.234	702	705	709	rBV2	30809	31615	1.82%	0.163%
6	6.363	723	727	738	rBV	1586863	1736253	100.00%	8.925%
7	6.486	744	748	754	rBV	1981364	1660285	95.62%	8.534%
8	6.539	754	757	763	rVB3	58131	74223	4.27%	0.382%
9	6.592	763	766	772	rVB3	30456	38119	2.20%	0.196%
10	6.716	783	787	793	rBV	1185493	1011685	58.27%	5.200%
11	6.869	809	813	821	rBV	1524053	1317417	75.88%	6.772%
12	6.981	828	832	837	rVB2	26997	36869	2.12%	0.190%
13	7.281	879	883	893	rBV	1010615	981476	56.53%	5.045%
14	7.392	900	902	910	rVB8	16733	30632	1.76%	0.157%
15	7.928	989	993	998	rBV	302698	279695	16.11%	1.438%
16	7.975	999	1001	1002	rBV	42038	30296	1.74%	0.156%
17	7.998	1002	1005	1008	rBV	1451424	1162748	66.97%	5.977%
18	8.351	1061	1065	1073	rBV3	77092	115088	6.63%	0.592%
19	8.586	1102	1105	1110	rVB	59250	58730	3.38%	0.302%
20	8.716	1123	1127	1133	rBV	82787	102564	5.91%	0.527%
21	8.792	1137	1140	1154	rVB2	151698	282641	16.28%	1.453%
22	9.016	1175	1178	1181	rVB2	29040	29179	1.68%	0.150%
23	9.075	1184	1188	1195	rVV	1692139	1496873	86.21%	7.694%
24	9.151	1198	1201	1203	rVV	79811	73613	4.24%	0.378%
25	9.175	1203	1205	1210	rVB2	42181	38542	2.22%	0.198%
26	9.222	1210	1213	1215	rBV2	37168	28467	1.64%	0.146%
27	9.345	1229	1234	1238	rBV4	41475	71170	4.10%	0.366%
28	9.410	1242	1245	1248	rVV2	70462	69382	4.00%	0.357%
29	9.469	1252	1255	1259	rVB	226315	191168	11.01%	0.983%
30	9.563	1269	1271	1275	rVB4	35552	38020	2.19%	0.195%
31	9.616	1277	1280	1284	rVB	130969	117947	6.79%	0.606%
32	9.674	1288	1290	1293	rVB	82393	68750	3.96%	0.353%
33	9.751	1300	1303	1307	rVV	1151941	992820	57.18%	5.103%
34	9.786	1307	1309	1313	rVB	57782	54817	3.16%	0.282%

LSC Area Percent Report

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Acq On : 29 Jan 2018 14:36
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Sample : J1253-19 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-10(0-5)

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.857	1318	1321	1323	rBV3	22094	30256	1.74%	0.156%
36	9.910	1327	1330	1332	rBV3	24283	30482	1.76%	0.157%
37	9.963	1336	1339	1342	rVV2	51419	51708	2.98%	0.266%
38	9.998	1342	1345	1348	rVB3	39008	39600	2.28%	0.204%
39	10.151	1368	1371	1373	rBV3	41327	49160	2.83%	0.253%
40	10.174	1373	1375	1378	rVB	114052	92354	5.32%	0.475%
41	10.298	1394	1396	1402	rVB2	38397	52578	3.03%	0.270%
42	10.398	1410	1413	1415	rVB	37310	31513	1.82%	0.162%
43	10.545	1435	1438	1447	rBV	654678	675208	38.89%	3.471%
44	10.651	1453	1456	1464	rBV2	124298	197768	11.39%	1.017%
45	10.739	1469	1471	1474	rBV3	37404	34701	2.00%	0.178%
46	11.098	1530	1532	1534	rBV	72365	55428	3.19%	0.285%
47	11.239	1553	1556	1558	rBV	926744	847583	48.82%	4.357%
48	11.263	1558	1560	1563	rVV	496932	405287	23.34%	2.083%
49	11.316	1567	1569	1572	rVV	131204	112962	6.51%	0.581%
50	11.798	1649	1651	1653	rBV	175086	127590	7.35%	0.656%
51	12.457	1760	1763	1767	rBV	642546	619857	35.70%	3.186%
52	12.686	1800	1802	1809	rVB	537978	566213	32.61%	2.910%
53	12.827	1823	1826	1829	rBV	944379	799076	46.02%	4.107%
54	13.892	2005	2007	2010	rVB2	600696	594782	34.26%	3.057%

Sum of corrected areas: 19454495

LSC Report - Integrated Chromatogram

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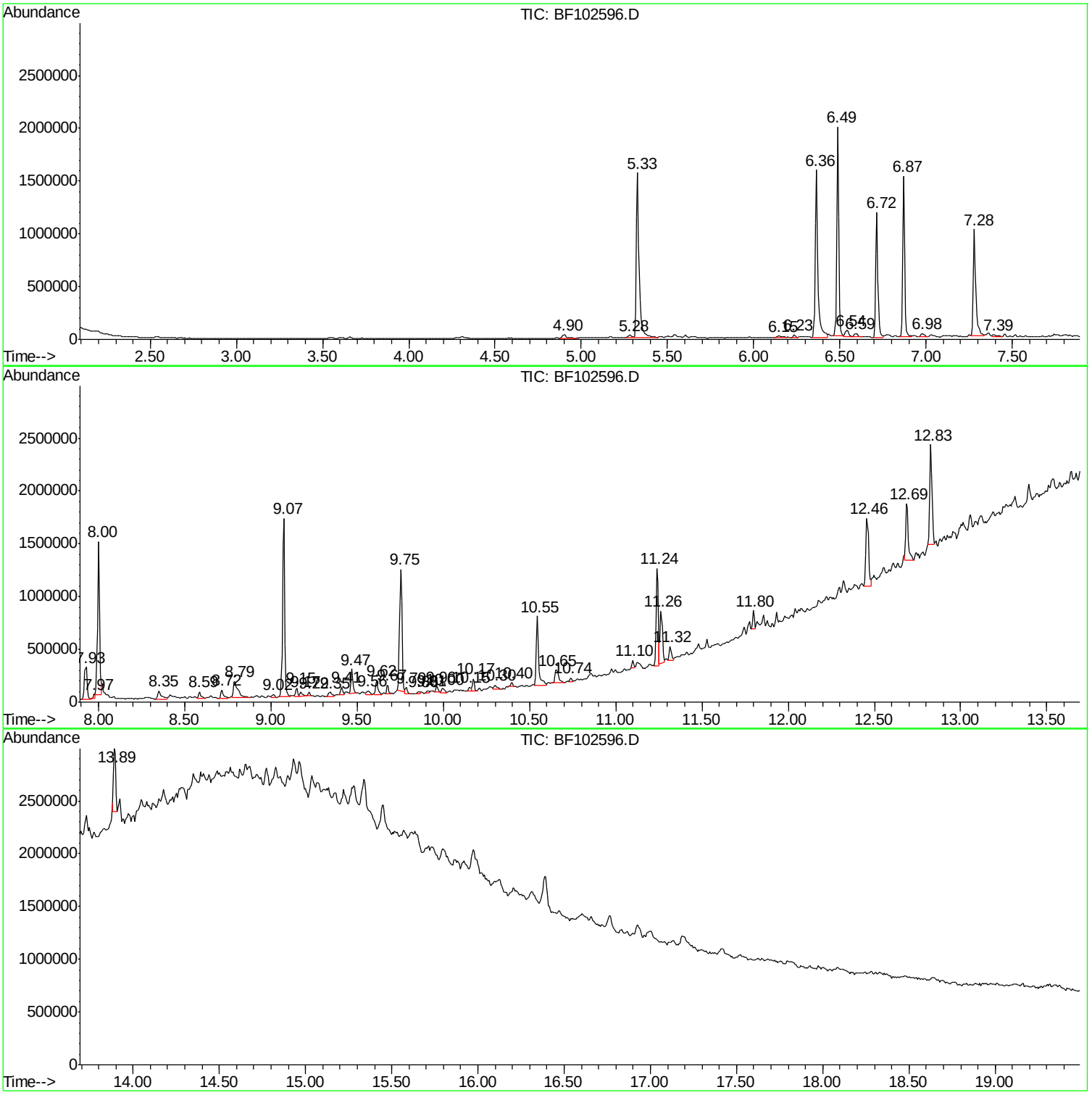
Data File : BF102596.D
Acq On : 29 Jan 2018 14:36
Operator : SJ/JU
Sample : J1253-19 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-10(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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\BF012918\
Data File : BF102596.D
Acq On : 29 Jan 2018 14:36
Operator : SJ/JU
Sample : J1253-19 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-10(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

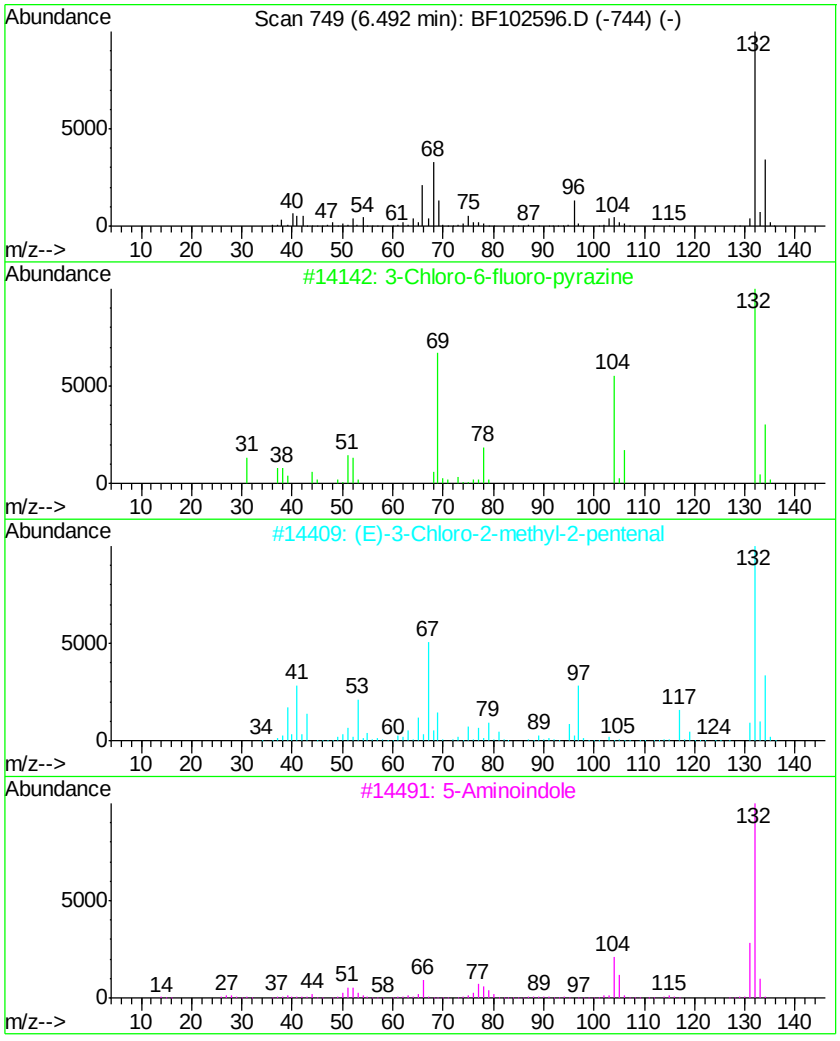
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

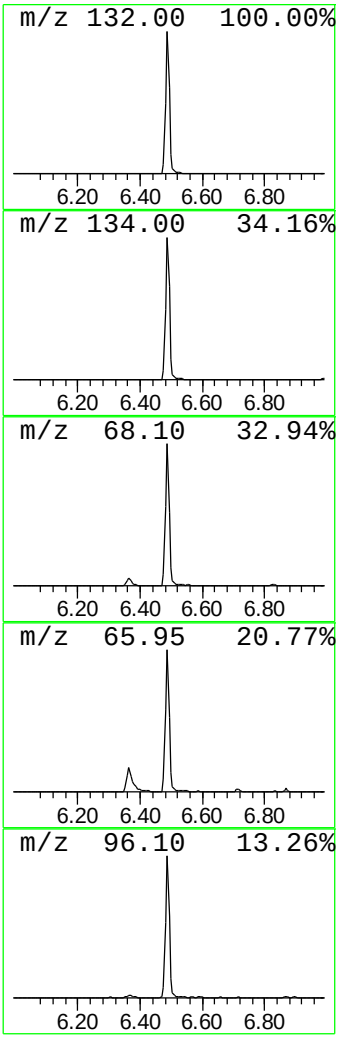
****

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	32.82 ng	1660290	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102596.D
Acq On : 29 Jan 2018 14:36
Operator : SJ/JU
Sample : J1253-19 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-10(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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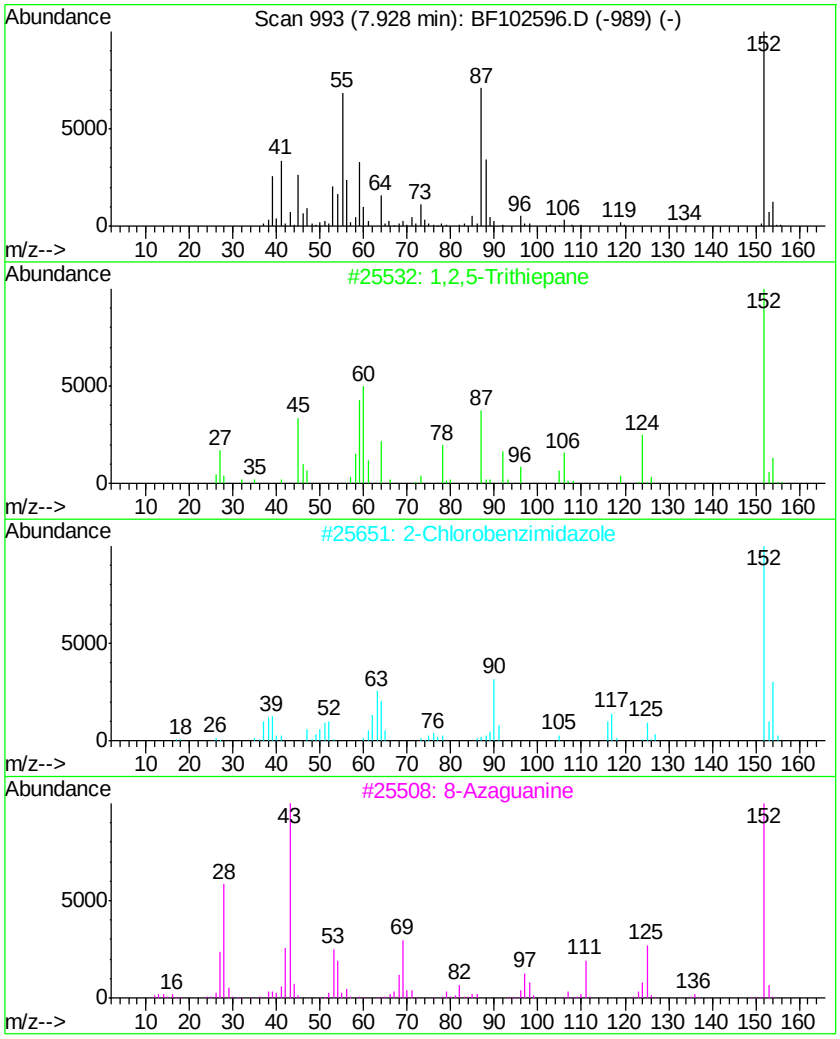
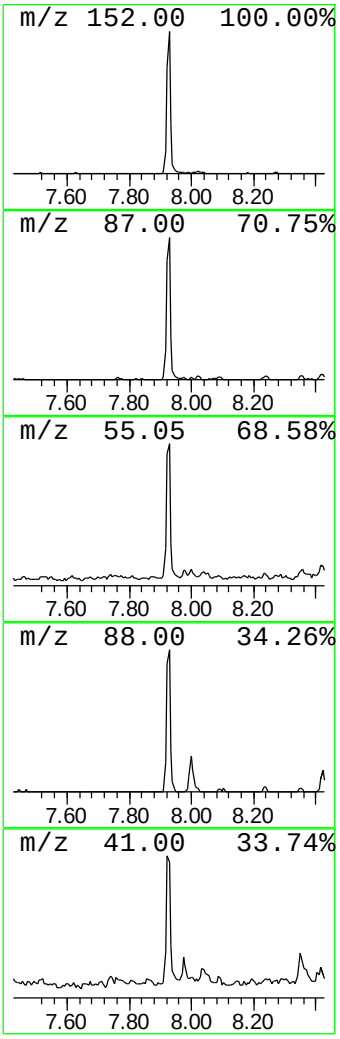
Peak Number 3 unknown7.93 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	4.81 ng	279695	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	47
2	2-Chlorobenzimidazole	152	C7H5ClN2	004857-06-1	27
3	8-Azaguanine	152	C4H4N6O	000134-58-7	22
4	trans-O-Dithiane-4,5-diol	152	C4H8O2S2	014193-38-5	17
5	2-Heptenoic acid, methyl ester, ...	142	C8H14O2	038693-91-3	12





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
Data File : BF102596.D
Acq On : 29 Jan 2018 14:36
Operator : SJ/JU
Sample : J1253-19 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-10(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

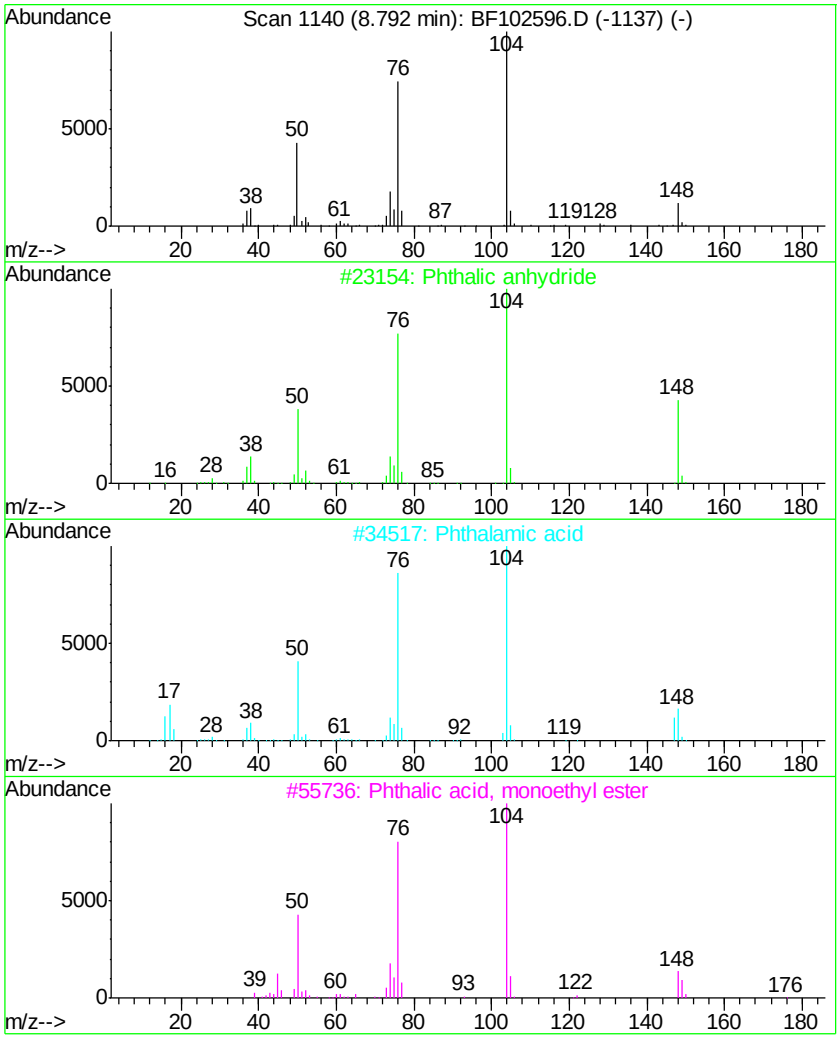
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

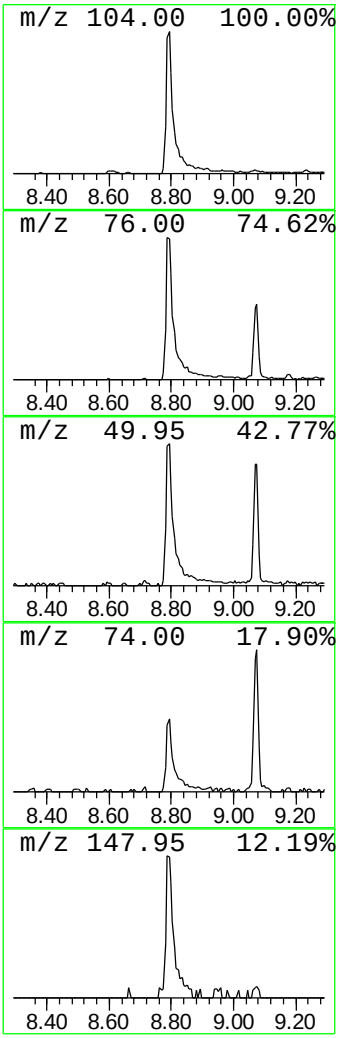
****

Peak Number 4 Phthalic anhydride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	4.86 ng	282641	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	Phthalamic acid	165	C8H7NO3	000088-97-1	90
3	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	90
4	Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	86
5	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
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Acq On : 29 Jan 2018 14:36
Operator : SJ/JU
Sample : J1253-19 2X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-10(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

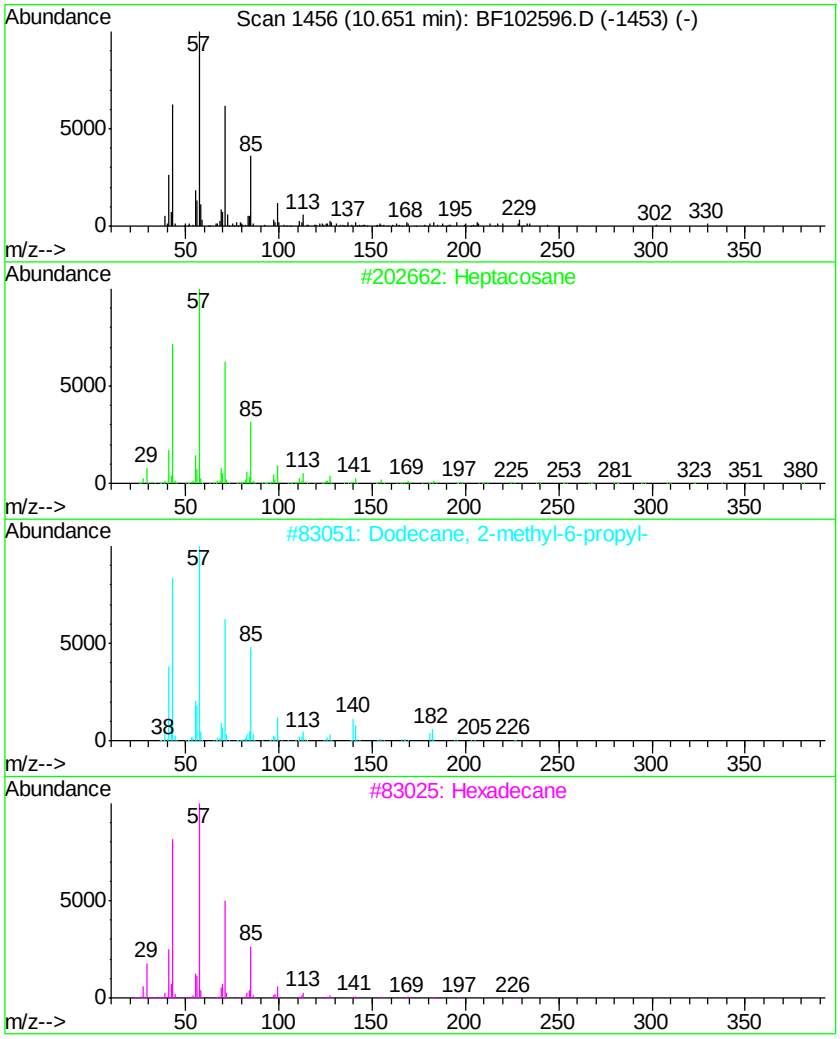
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

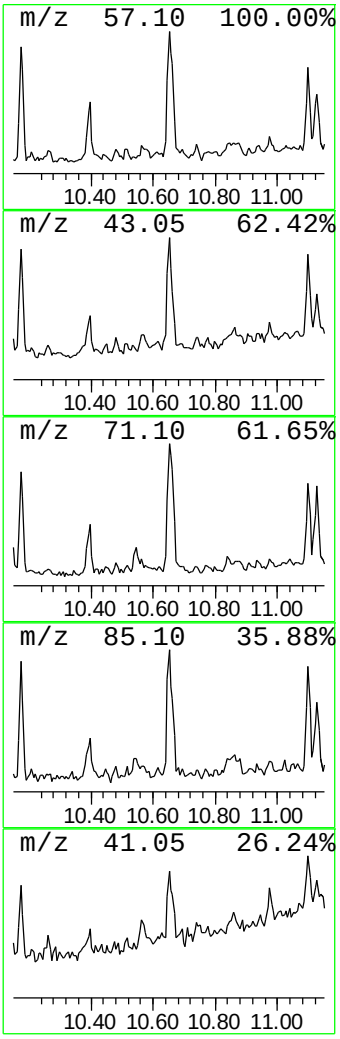
****

Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.67 ng	197768	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Hexadecane	226	C16H34	000544-76-3	80
4	Eicosane	282	C20H42	000112-95-8	80
5	Docosane	310	C22H46	000629-97-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012918\
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Acq On : 29 Jan 2018 14:36
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Misc :
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Instrument : BNA_F
ClientSampleId : WC-10(0-5)

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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
unknown6.49	6.49	32.8	ng	1660290	1	6.72	1011690	20.0
unknown7.93	7.93	4.8	ng	279695	2	8.00	1162750	20.0
Phthalic anhydride	8.79	4.9	ng	282641	2	8.00	1162750	20.0
Heptacosane	10.65	4.7	ng	197768	4	11.24	847583	20.0