Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100980.D
Acq On : 29 Nov 2017 16:17
Operator : SJ/JU
Sample : I6304-26 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112817-C

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-BF110817.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	5.069	503	507	514	rBV	38660	45072	5.20%	0.548%
2	5.463	570	574	578	rBV	722093	680867	78.53%	8.285%
3	6.481	742	747	756	rBV	748081	710466	81.95%	8.645%
4	6.622	767	771	774	rBV	815738	737700	85.09%	8.977%
5	6.851	806	810	813	rBV	485258	383963	44.29%	4.672%
6	7.004	833	836	840	rBV	665892	576621	66.51%	7.017%
7	7.410	901	905	909	rBV	466121	426302	49.17%	5.188%
8	8.134	1024	1028	1031	rBV	636108	496395	57.26%	6.040%
9	9.204	1207	1210	1214	rVB	987637	866970	100.00%	10.550%
10	9.281	1220	1223	1226	rVB	14428	10468	1.21%	0.127%
11	9.598	1274	1277	1280	rBV	74115	56425	6.51%	0.687%
12	9.810	1309	1313	1317	rVB	33381	27348	3.15%	0.333%
13	9.886	1323	1326	1330	rVB	542257	500879	57.77%	6.095%
14	10.310	1395	1398	1401	rVB	34202	25804	2.98%	0.314%
15	10.675	1457	1460	1464	rBV	484864	403723	46.57%	4.913%
16	10.780	1475	1478	1489	rVB2	22678	28984	3.34%	0.353%
17	11.375	1575	1579	1582	rBV	490625	418948	48.32%	5.098%
18	11.398	1582	1583	1586	rVB	39641	23495	2.71%	0.286%
19	11.892	1663	1667	1672	rBV2	25802	34190	3.94%	0.416%
20	11.986	1681	1683	1686	rBV2	9711	10183	1.17%	0.124%
21	12.586	1782	1785	1790	rVB	82271	72719	8.39%	0.885%
22	12.686	1798	1802	1806	rBV5	8497	12498	1.44%	0.152%
23	12.822	1819	1825	1828	rBV2	62910	76613	8.84%	0.932%
24	12.874	1831	1834	1838	rVB6	8585	10809	1.25%	0.132%
25	12.957	1844	1848	1852	rVB	731106	598612	69.05%	7.284%
26	13.033	1856	1861	1862	rBV5	8978	12446	1.44%	0.151%
27	13.145	1877	1880	1883	rVB2	12630	15718	1.81%	0.191%
28	13.374	1917	1919	1922	rBV4	7577	11143	1.29%	0.136%
29	13.521	1940	1944	1947	rBV6	10097	14948	1.72%	0.182%
30	13.845	1996	1999	2005	rBV2	70025	77331	8.92%	0.941%
31	14.016	2024	2028	2031	rBV	451139	434484	50.12%	5.287%
32	15.492	2274	2279	2283	rBV	256161	330081	38.07%	4.017%
33	16.180	2393	2396	2404	rVB8	40888	85588	9.87%	1.041%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100980.D
Acq On : 29 Nov 2017 16:17
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Sample : I6304-26 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112817-C

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

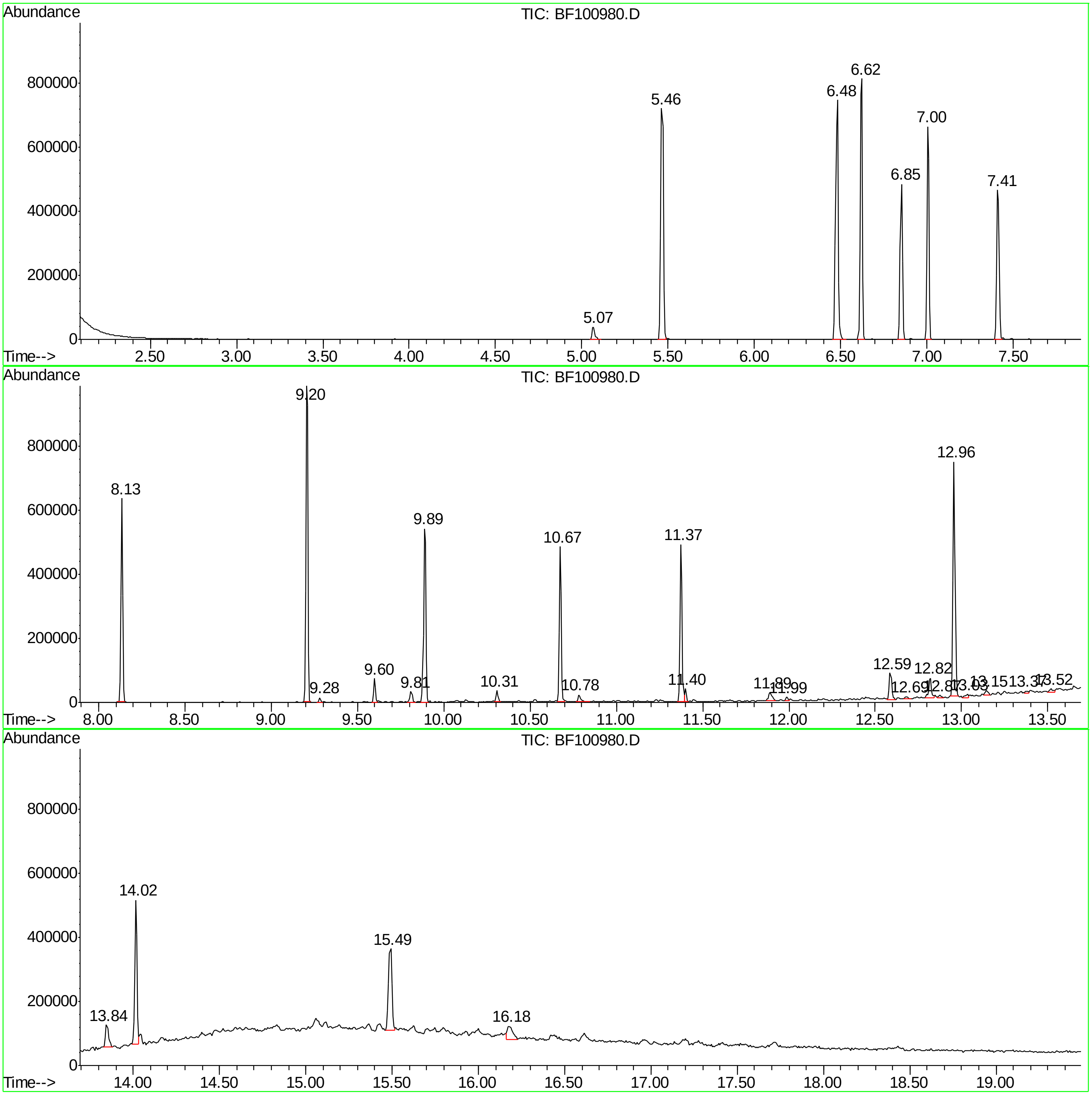
Sum of corrected areas: 8217793

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100980.D
Acq On : 29 Nov 2017 16:17
Operator : SJ/JU
Sample : I6304-26 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112817-C

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.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\BF112917\
Data File : BF100980.D
Acq On : 29 Nov 2017 16:17
Operator : SJ/JU
Sample : I6304-26 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112817-C

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.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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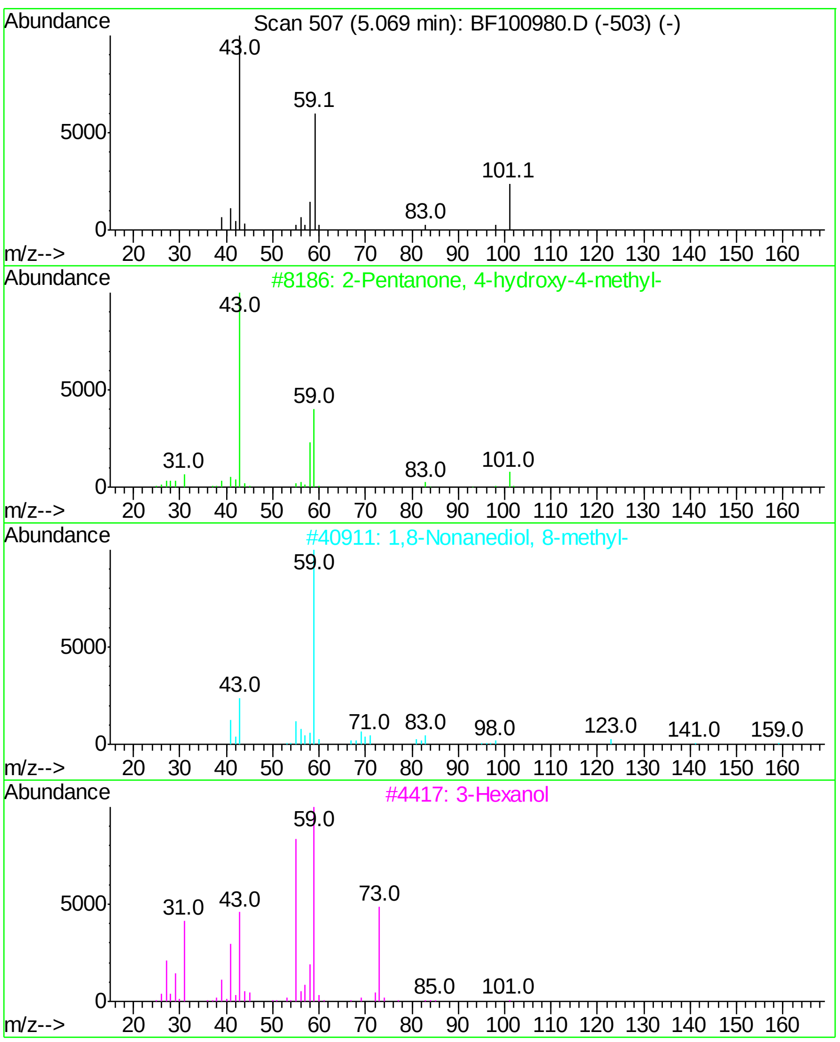
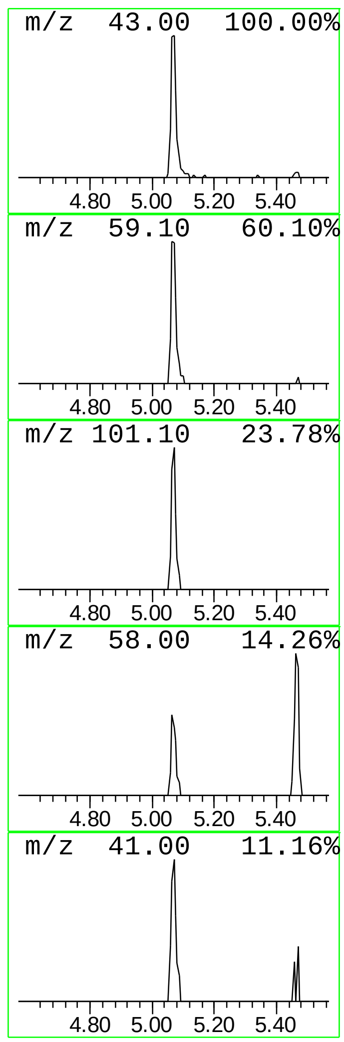
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	2.35 ng	45072	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	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	37
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100980.D
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Operator : SJ/JU
Sample : I6304-26 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112817-C

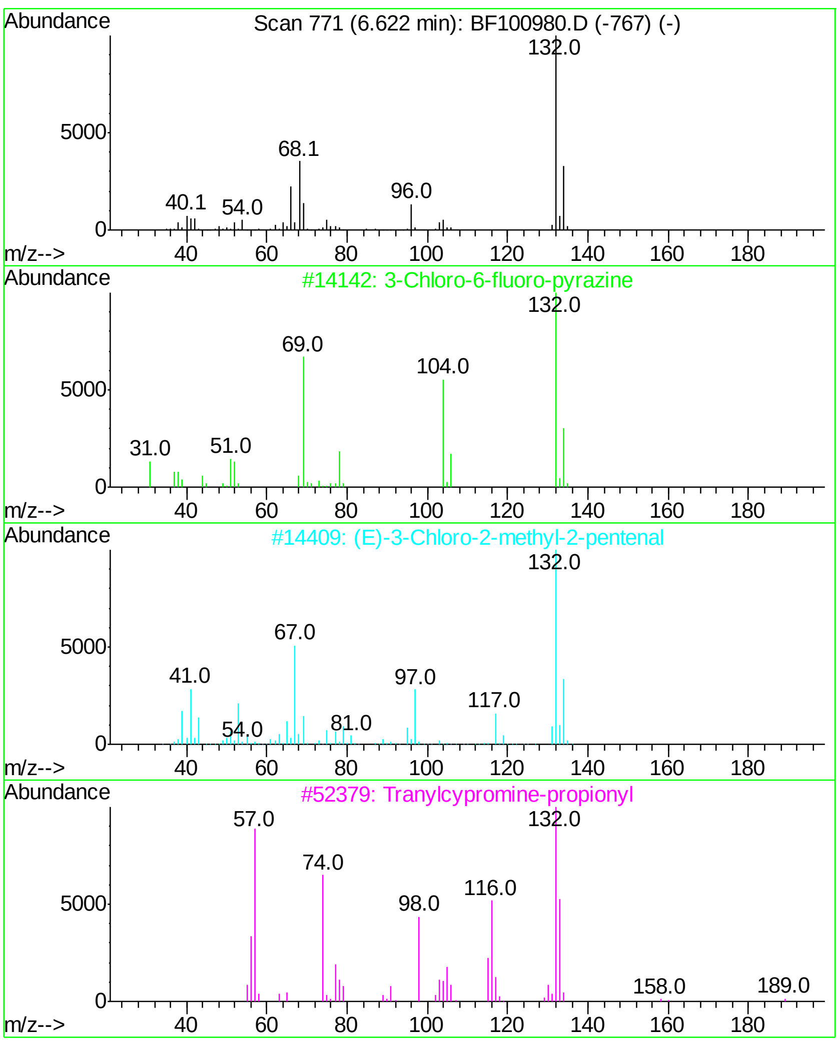
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

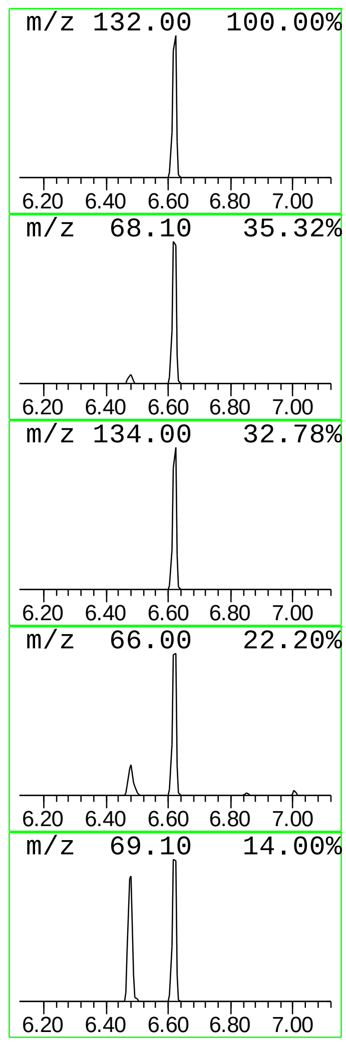
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	38.43 ng	737700	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	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Xenon	132	Xe	007440-63-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112917\
Data File : BF100980.D
Acq On : 29 Nov 2017 16:17
Operator : SJ/JU
Sample : I6304-26 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-C

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.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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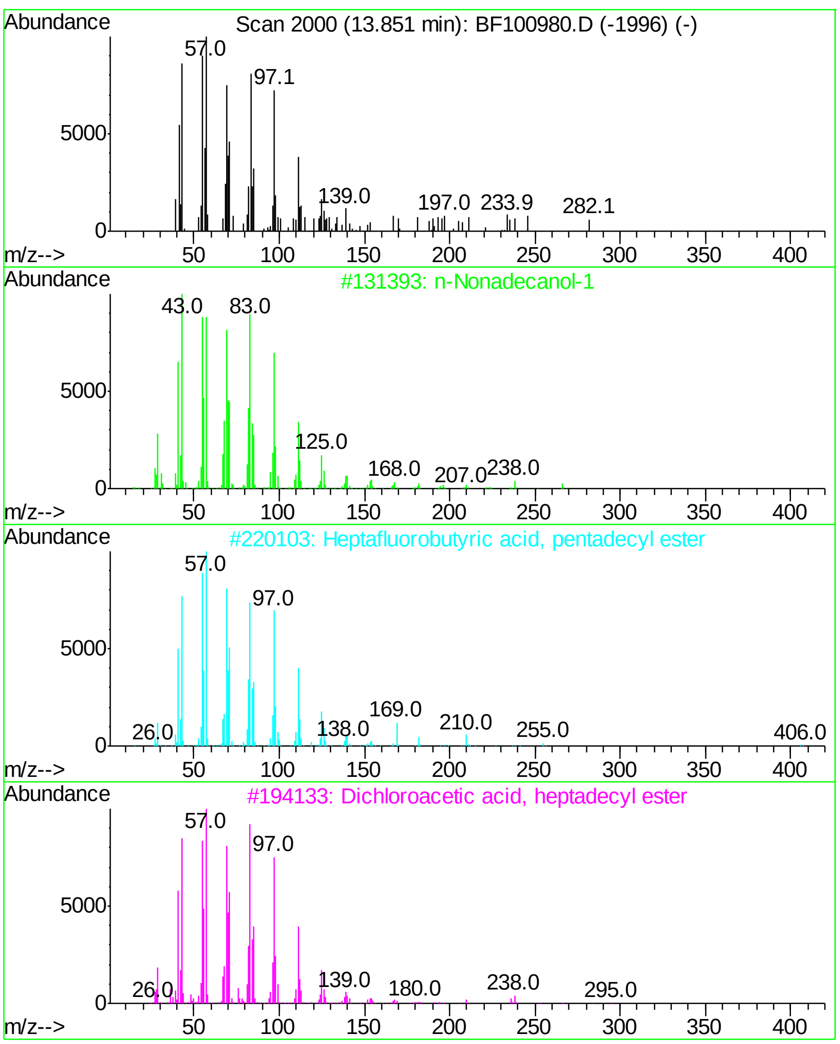
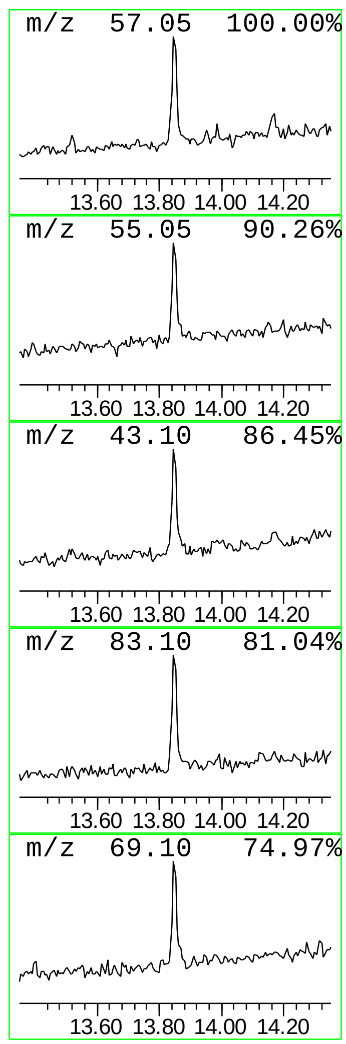
Peak Number 4 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.56 ng	77331	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





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Acq On : 29 Nov 2017 16:17
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Sample : I6304-26 2X
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-112817-C

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.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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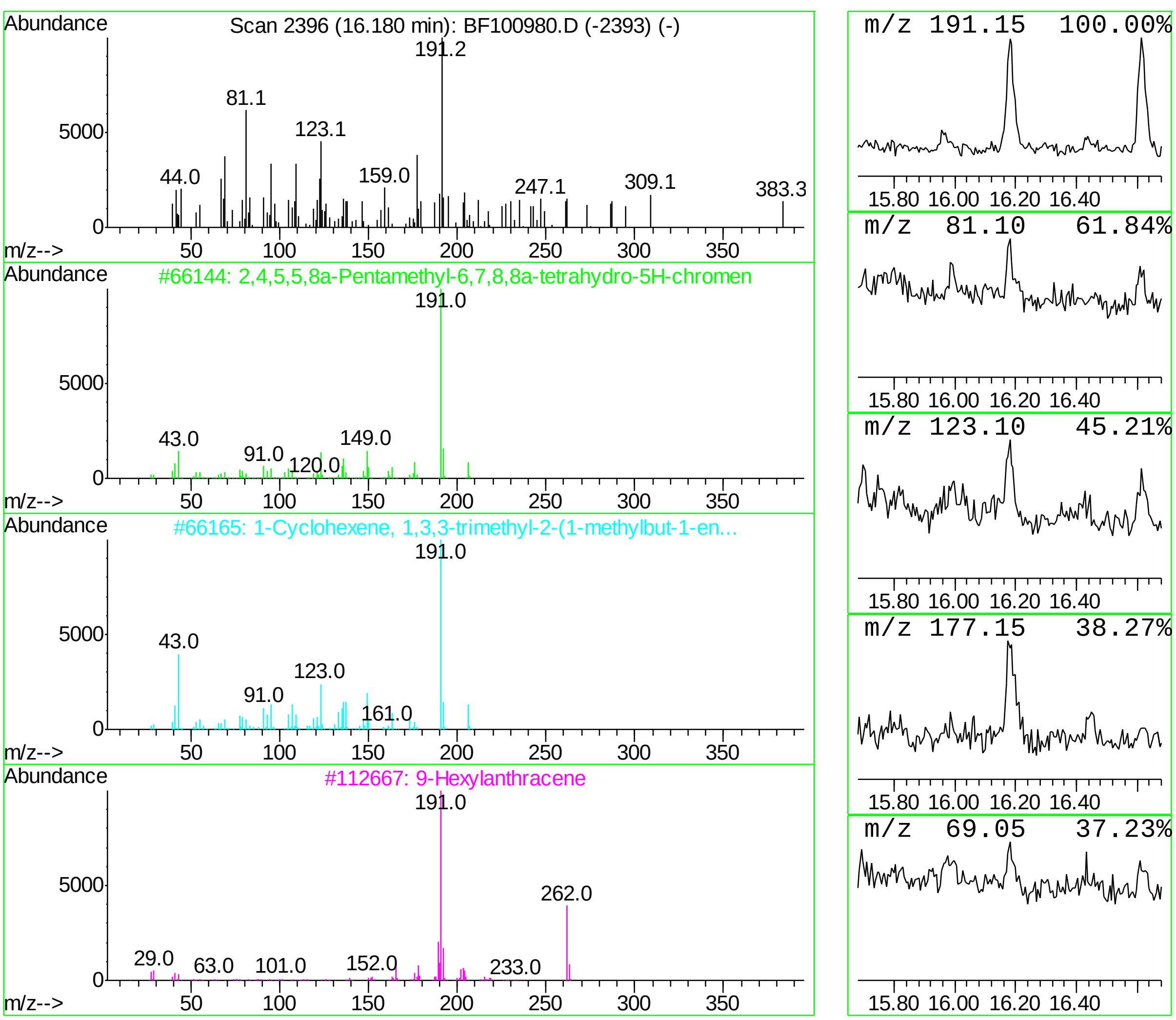
Peak Number 5 unknown16.18 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	5.19 ng	85588	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	35
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	32
3	9-Hexylanthracene	262	C20H22	033576-55-5	30
4	Isophthalic acid, hex-4-yn-3-yl ...	288	C17H20O4	1000343-83-8	27
5	1H-Pyrrolo[3,4-c]pyridine-1,3,(2...	191	C9H9N3O2	298688-32-1	25



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112917\
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Acq On : 29 Nov 2017 16:17
Operator : SJ/JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CL-02-112817-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.07	2.4	ng	45072	1	6.85	383963	20.0
unknown6.62	6.62	38.4	ng	737700	1	6.85	383963	20.0
n-Nonadecanol-1	13.85	3.6	ng	77331	5	14.02	434484	20.0
unknown16.18	16.18	5.2	ng	85588	6	15.49	330081	20.0