LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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	5.201	484	487	493	rVB	94748	101268	3.35%	0.429%
2	5.613	554	557	565	rBV	1499765	1358075	44.92%	5.760%
3	6.613	723	727	732	rBV	929945	855359	28.29%	3.628%
4	6.748	745	750	753	rBV	2479828	2321538	76.79%	9.846%
5	6.966	783	787	791	rBV	862468	696809	23.05%	2.955%
6	7.125	809	814	817	rBV	2379662	2165878	71.64%	9.185%
7	7.484	871	875	878	rBV	63706	56533	1.87%	0.240%
8	7.531	878	883	886	rBV	1831546	1977086	65.39%	8.385%
9	7.584	889	892	897	rVV	72890	73851	2.44%	0.313%
10	7.625	897	899	902	rVB	48631	38329	1.27%	0.163%
11	7.901	942	946	952	rBV	284520	298298	9.87%	1.265%
12	8.101	976	980	984	rBV3	33019	42265	1.40%	0.179%
13	8.178	990	993	995	rBV	43754	31387	1.04%	0.133%
14	8.248	1001	1005	1010	rBV	1025504	852402	28.19%	3.615%
15	8.660	1071	1075	1080	rBV	229252	251066	8.30%	1.065%
16	8.719	1083	1085	1089	rVB4	32297	34884	1.15%	0.148%
17	8.907	1113	1117	1120	rBV3	36371	46271	1.53%	0.196%
18	9.078	1143	1146	1153	rVB	47710	57219	1.89%	0.243%
19	9.325	1183	1188	1191	rBV	3168579	3023389	100.00%	12.822%
20	9.425	1202	1205	1209	rVB	53005	47976	1.59%	0.203%
21	9.566	1225	1229	1232	rBV4	22171	34546	1.14%	0.147%
22	9.672	1242	1247	1251	rBV2	170465	220637	7.30%	0.936%
23	9.713	1251	1254	1257	rVB	191105	154524	5.11%	0.655%
24	9.854	1275	1278	1281	rBV4	25516	33147	1.10%	0.141%
25	9.913	1285	1288	1291	rBV2	59197	64856	2.15%	0.275%
26	10.007	1299	1304	1313	rBV	1005083	927814	30.69%	3.935%
27	10.166	1328	1331	1334	rBV4	27239	37594	1.24%	0.159%
28	10.207	1336	1338	1340	rVV3	55444	52608	1.74%	0.223%
29	10.231	1340	1342	1346	rVB4	56002	59852	1.98%	0.254%
30	10.313	1353	1356	1361	rBV3	81641	128558	4.25%	0.545%
31	10.366	1363	1365	1367	rBV2	54834	47472	1.57%	0.201%
32	10.389	1367	1369	1372	rVV2	153525	139598	4.62%	0.592%
33	10.419	1372	1374	1379	rVB4	60434	57503	1.90%	0.244%
34	10.578	1398	1401	1404	rBV4	27675	32181	1.06%	0.136%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
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Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.801	1435	1439	1444	rVB	1694617	1600301	52.93%	6.787%
36	10.889	1451	1454	1460	rBV	208600	181879	6.02%	0.771%
37	10.972	1466	1468	1470	rBV2	52602	59810	1.98%	0.254%
38	11.001	1471	1473	1477	rVB3	81930	91327	3.02%	0.387%
39	11.042	1477	1480	1482	rBV2	60637	54061	1.79%	0.229%
40	11.154	1497	1499	1503	rVB4	35834	41471	1.37%	0.176%
41	11.189	1503	1505	1507	rBV	45232	37871	1.25%	0.161%
42	11.342	1529	1531	1534	rBV2	31811	33376	1.10%	0.142%
43	11.378	1534	1537	1540	rVB4	37419	39445	1.30%	0.167%
44	11.501	1554	1558	1561	rBV	777268	693072	22.92%	2.939%
45	11.695	1588	1591	1596	rBV7	35507	53566	1.77%	0.227%
46	12.889	1791	1794	1798	rVB	42437	37030	1.22%	0.157%
47	13.083	1823	1827	1831	rBV	2629063	2715905	89.83%	11.518%
48	13.960	1973	1976	1982	rBV	114103	115146	3.81%	0.488%
49	14.148	2004	2008	2013	rVB	925620	814979	26.96%	3.456%
50	15.683	2264	2269	2275	rBV	538242	689396	22.80%	2.924%

Sum of corrected areas: 23579408

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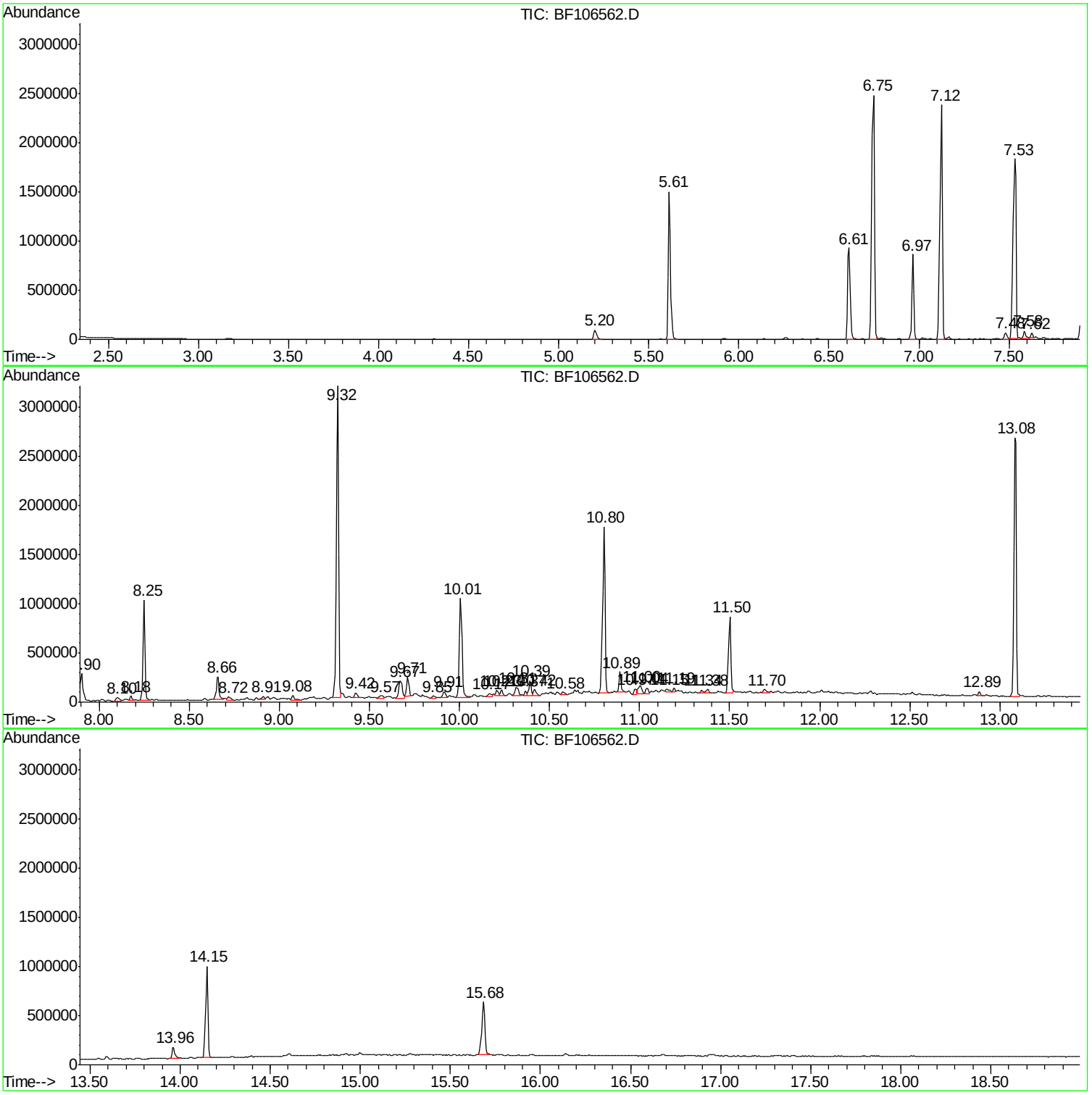
Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

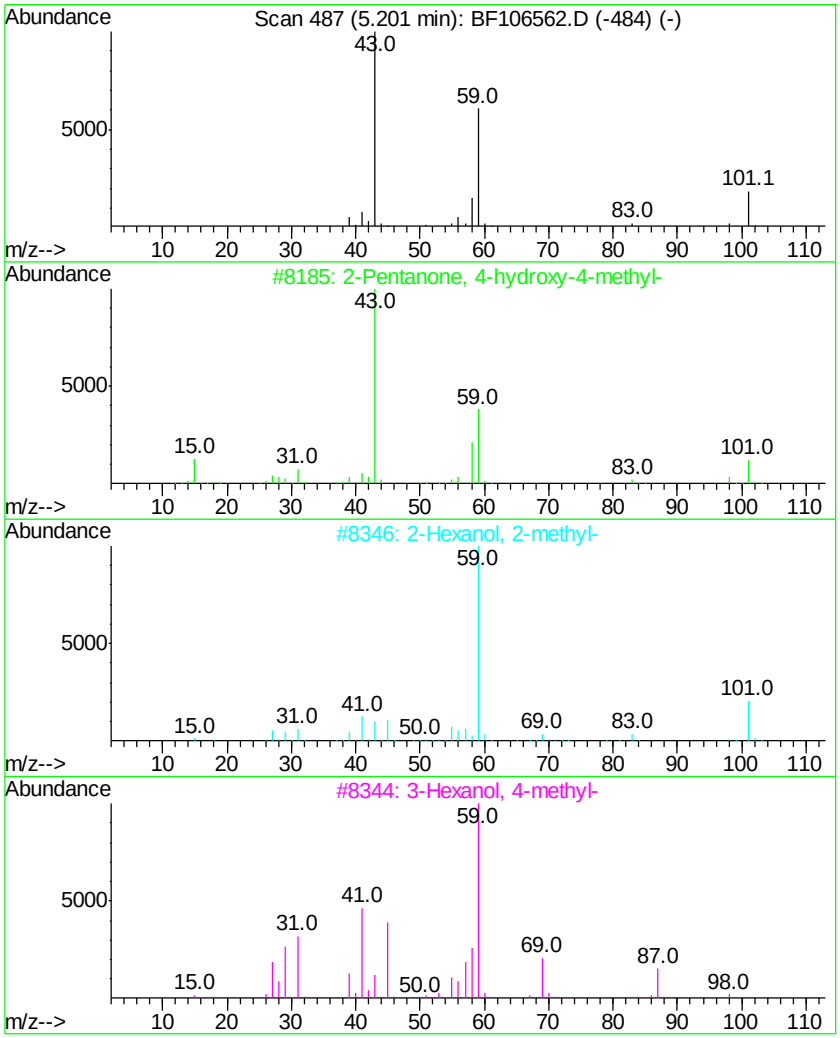
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

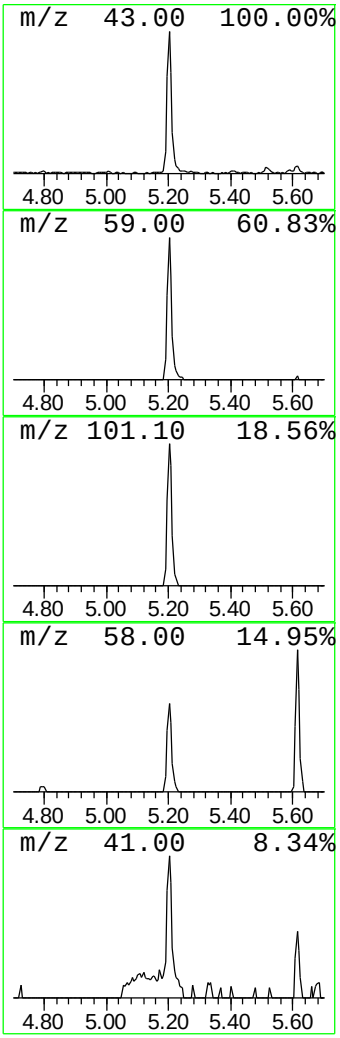
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.91 ng	101268	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Guanidine	59	CH5N3	000113-00-8	9





Library Search Compound Report

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Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

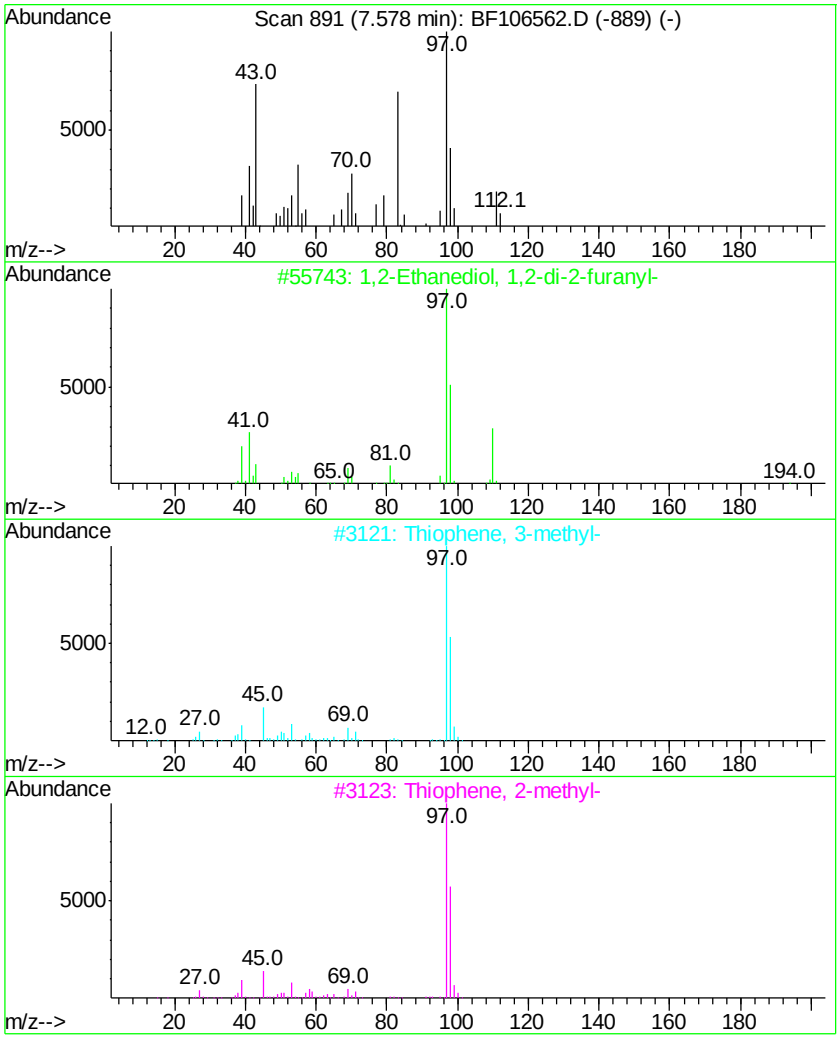
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

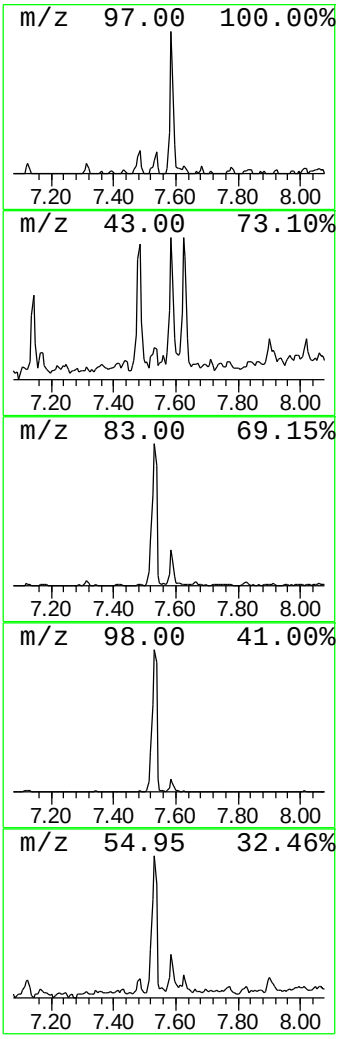
****

Peak Number 4 1,2-Ethanediol, 1,2-di-2-fu... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	2.12 ng	73851	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol, 1,2-di-2-furanyl-	194	C10H10O4	004464-77-1	50
2	Thiophene, 3-methyl-	98	C5H6S	000616-44-4	40
3	Thiophene, 2-methyl-	98	C5H6S	000554-14-3	40
4	1-Pentyne, 3-methoxy-3-methyl-	112	C7H12O	022802-35-3	38
5	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	37





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

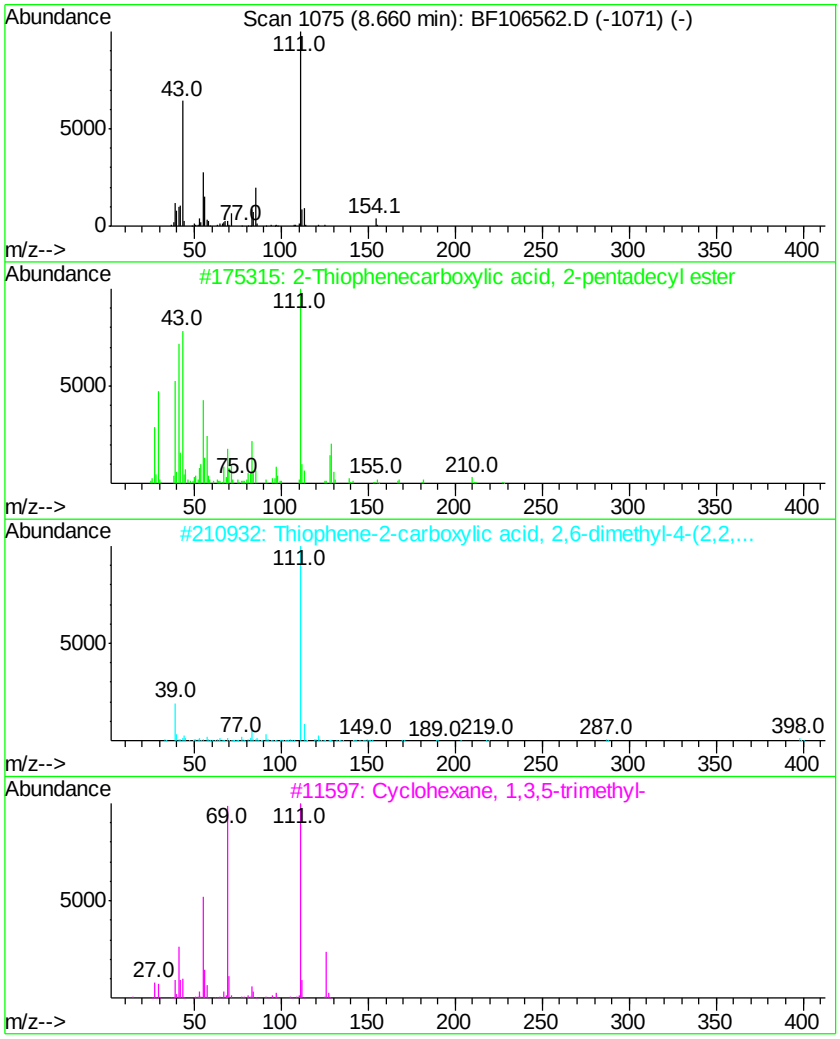
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

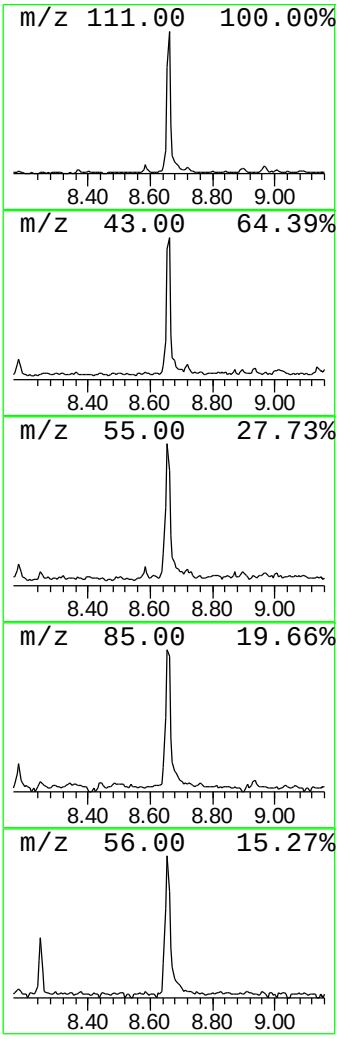
****

Peak Number 5 unknown8.66 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	5.89 ng	251066	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiophenecarboxylic acid, 2-pe...	338	C20H34O2S	1000280-66-4	45
2	Thiophene-2-carboxylic acid, 2,6...	398	C16H12F6O3S	1000304-48-8	38
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	36
4	Pyridin-2,6-diol, diacetate	195	C9H9NO4	1000153-09-2	33
5	Piperidine-2,5-dione	113	C5H7NO2	052065-78-8	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

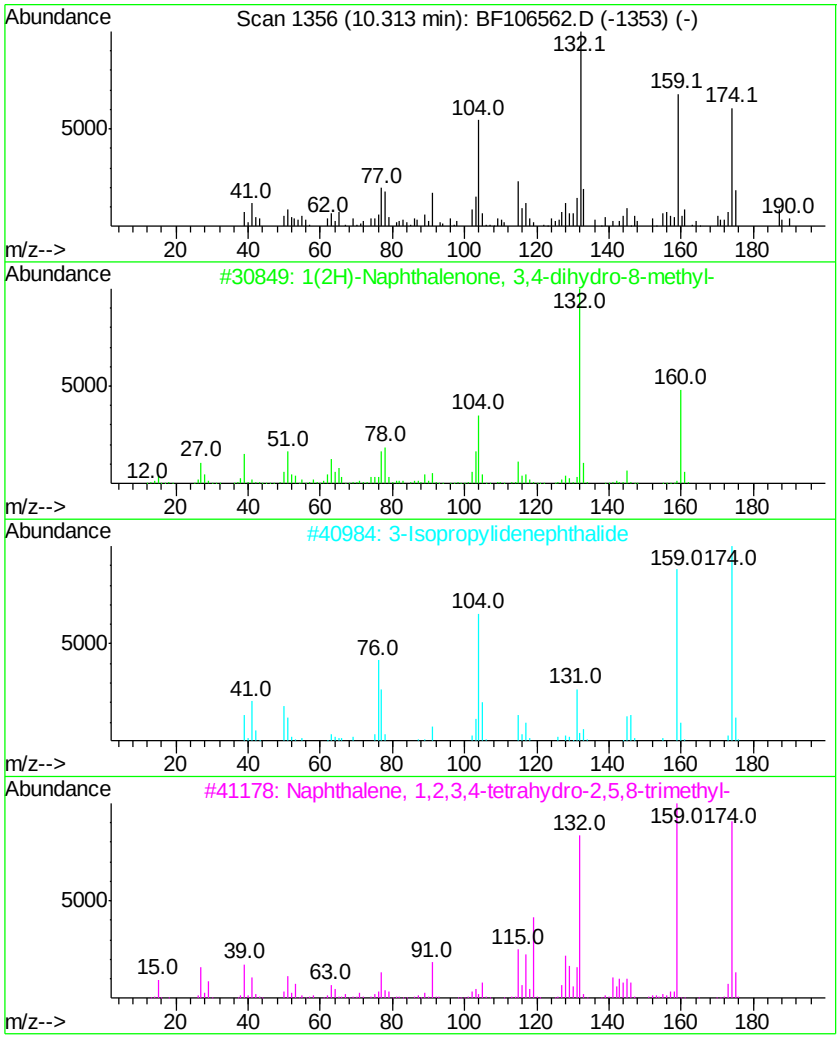
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

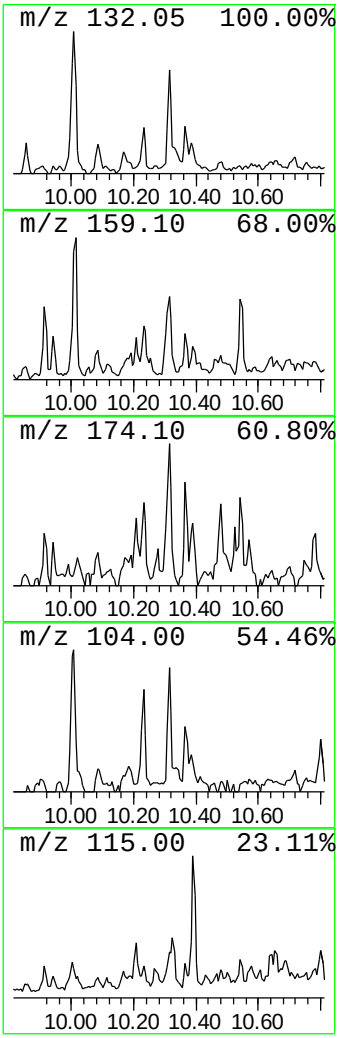
****

Peak Number 6 unknown10.31 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.31	2.77 ng	128558	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	051015-28-2	46
2	3-Isopropylidenephthalide	174	C11H10O2	004767-54-8	43
3	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-17-7	43
4	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	021693-55-0	42
5	Acrylophenone, 2,2',5'-trimethyl-	174	C12H14O	016205-96-2	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

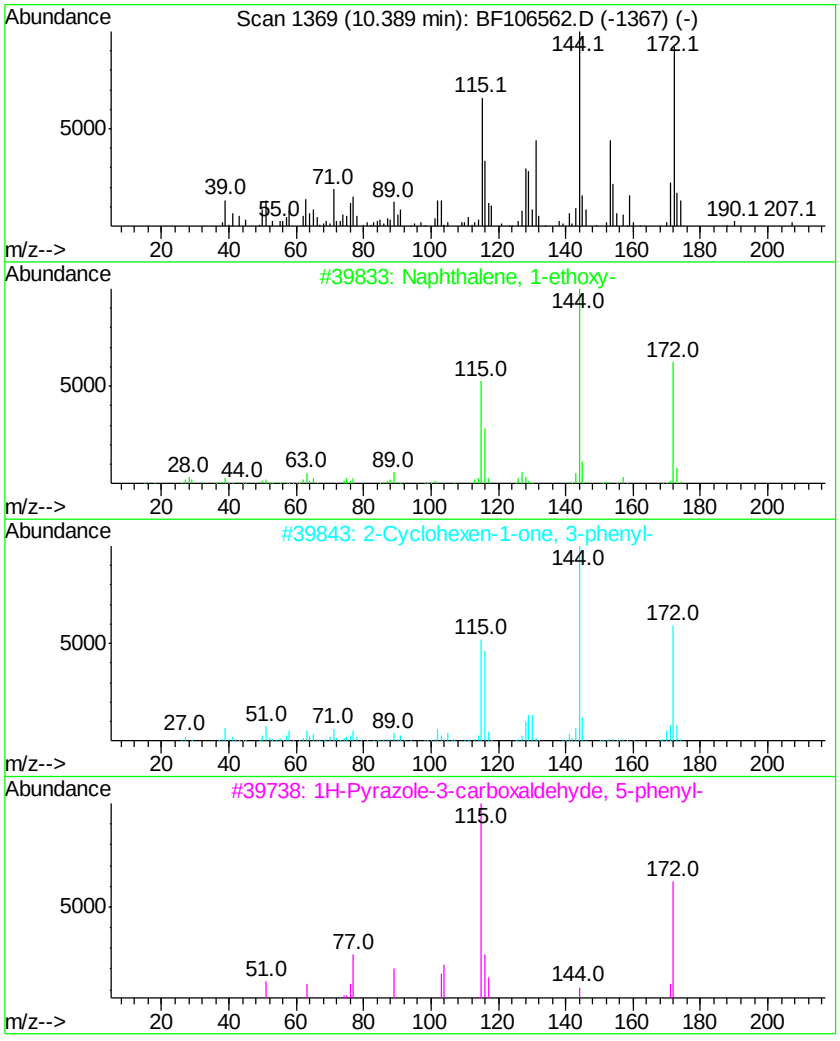
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

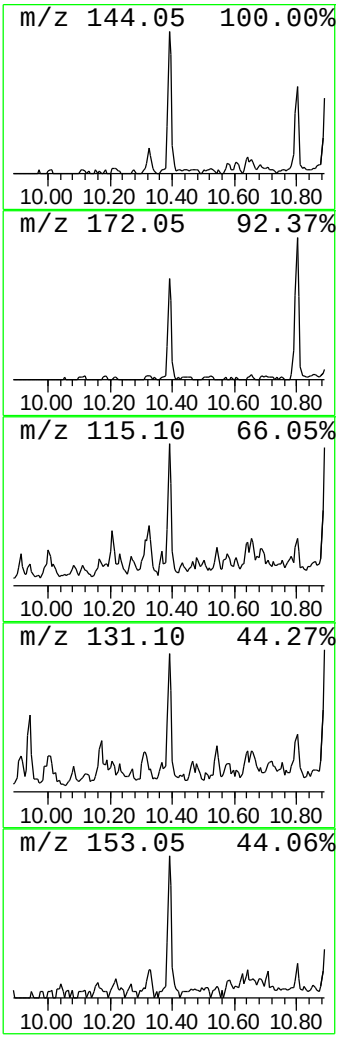
****

Peak Number 7 Naphthalene, 1-ethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.39	3.01 ng	139598	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-ethoxy-	172	C12H12O	005328-01-8	91
2	2-Cyclohexen-1-one, 3-phenyl-	172	C12H12O	010345-87-6	53
3	1H-Pyrazole-3-carboxaldehyde, 5-...	172	C10H8N2O	057204-65-6	49
4	Benzofuran, 3-methyl-2-(1-methyl...	172	C12H12O	023911-58-2	41
5	1-Naphthalenol	144	C10H8O	000090-15-3	38





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

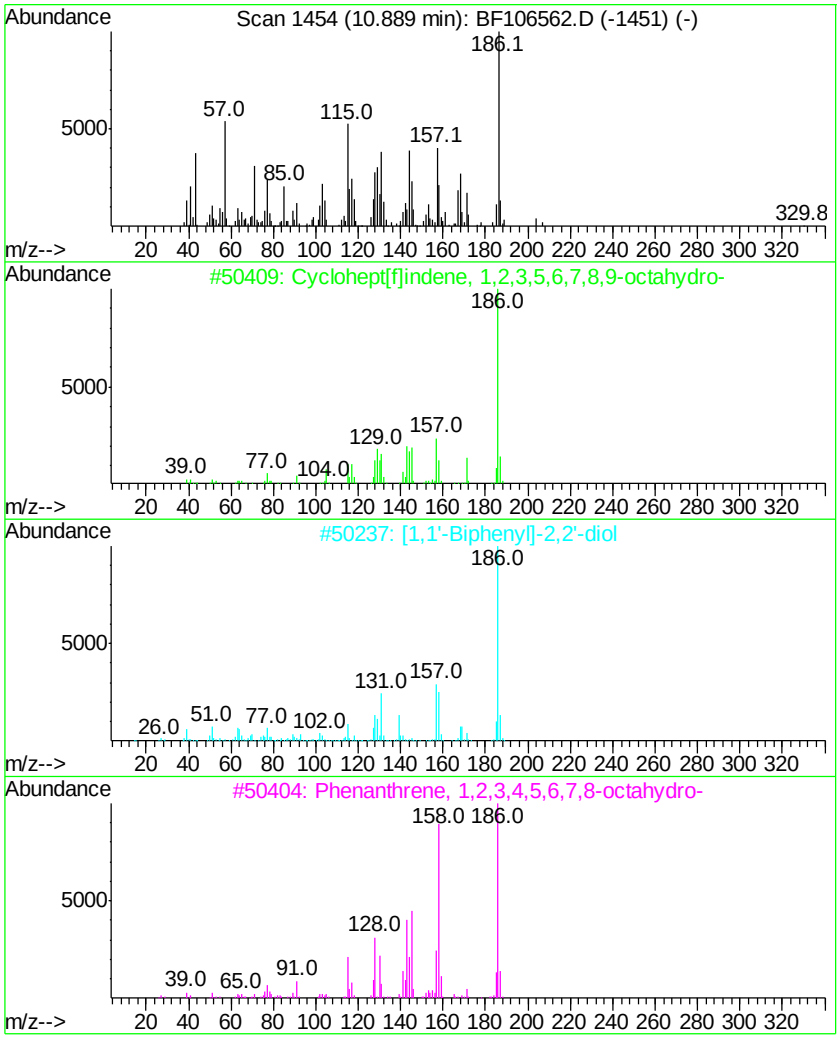
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

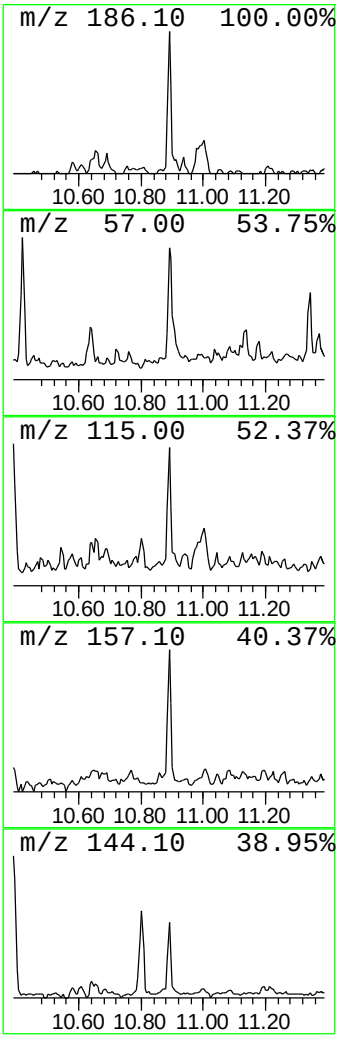
****

Peak Number 8 Cyclohept[f]indene, 1,2,3,5... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.89	5.25 ng	181879	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohept[f]indene, 1,2,3,5,6,7,...	186	C14H18	007140-25-2	58
2	[1,1'-Biphenyl]-2,2'-diol	186	C12H10O2	001806-29-7	55
3	Phenanthrene, 1,2,3,4,5,6,7,8-oc...	186	C14H18	005325-97-3	46
4	[1,1'-Biphenyl]-4,4'-diol	186	C12H10O2	000092-88-6	45
5	Phenol, 3-phenoxy-	186	C12H10O2	000713-68-8	43





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Data File : BF106562.D
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Sample : J3563-02
Misc :
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Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

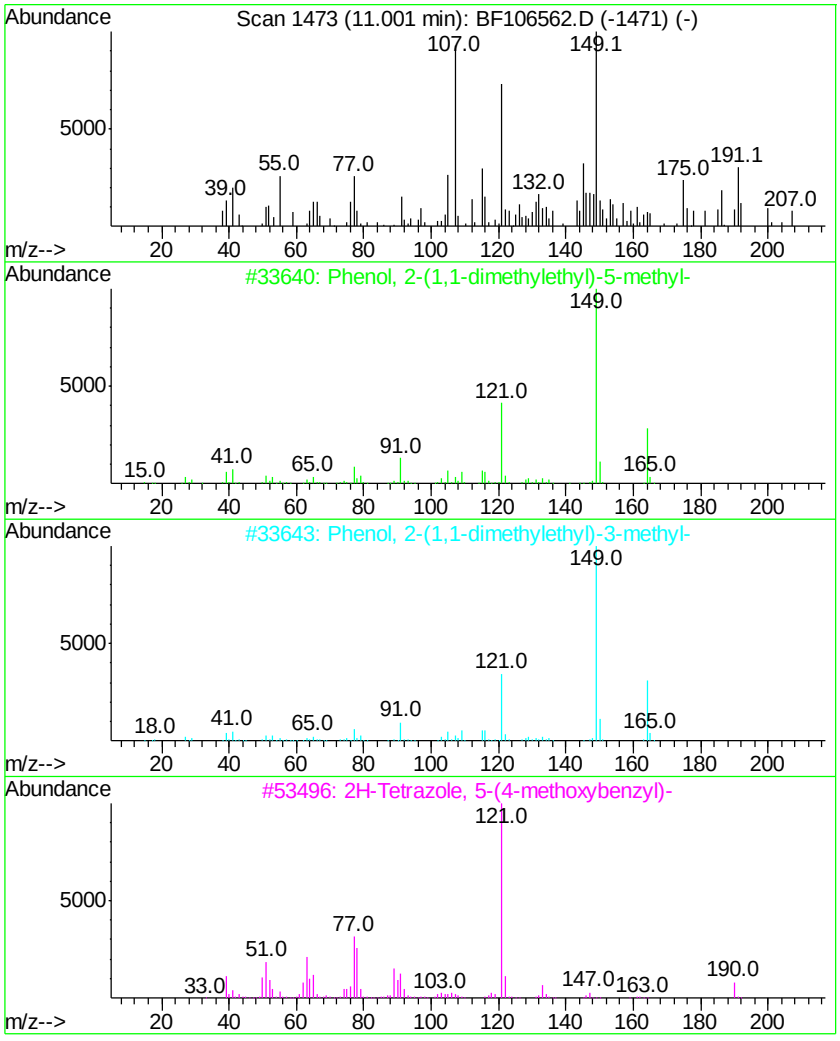
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

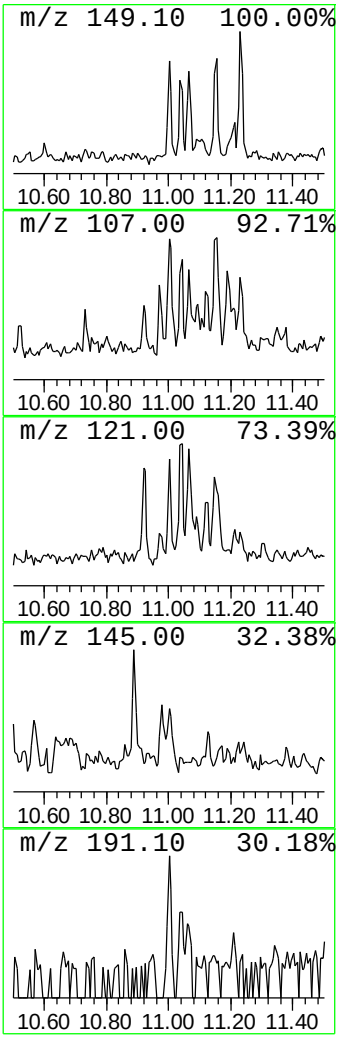
****

Peak Number 9 unknown11.00 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	2.64 ng	91327	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	46
2	Phenol, 2-(1,1-dimethylethyl)-3-...	164	C11H16O	013037-79-1	38
3	2H-Tetrazole, 5-(4-methoxybenzyl)-	190	C9H10N4O	1000315-87-6	25
4	Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	25
5	1,3-Cyclohexadiene, 1,5,5,6-tetr...	136	C10H16	000514-94-3	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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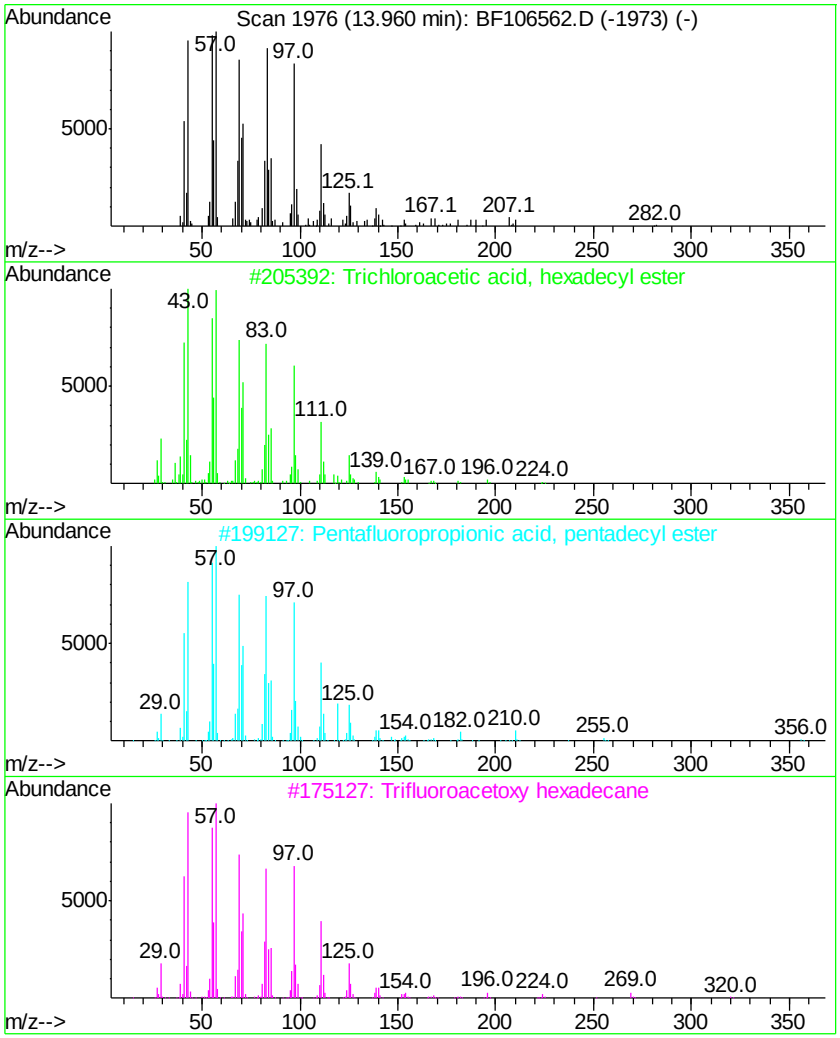
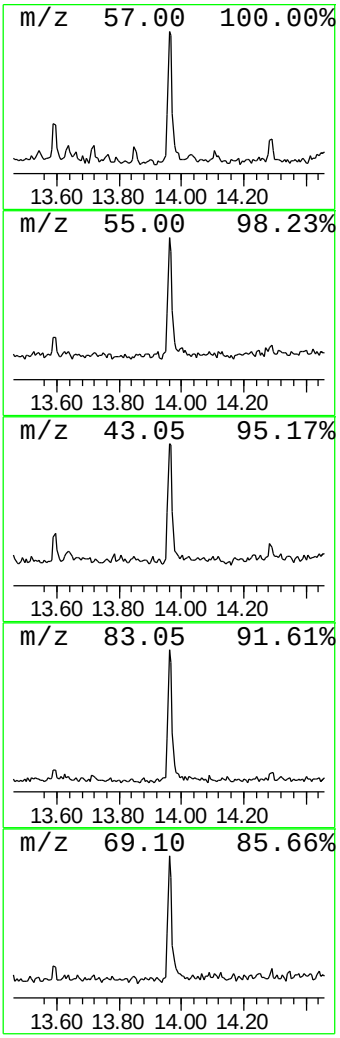
Peak Number 10 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	2.83 ng	115146	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061818\
Data File : BF106562.D
Acq On : 19 Jun 2018 2:49
Operator : JU/SJ
Sample : J3563-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.20	2.9	ng	101268	1	6.97	696809	20.0
1,2-Ethanediol, 1...	7.58	2.1	ng	73851	1	6.97	696809	20.0
unknown8.66	8.66	5.9	ng	251066	2	8.25	852402	20.0
unknown10.31	10.31	2.8	ng	128558	3	10.01	927814	20.0
Naphthalene, 1-et...	10.39	3.0	ng	139598	3	10.01	927814	20.0
Cyclohept[f]inden...	10.89	5.3	ng	181879	4	11.50	693072	20.0
unknown11.00	11.00	2.6	ng	91327	4	11.50	693072	20.0
Trichloroacetic a...	13.96	2.8	ng	115146	5	14.15	814979	20.0