LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099073.D
Acq On : 4 Oct 2017 18:11
Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

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-BF092317.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	2.157	7	12	18	rVB	599378	756592	18.67%	2.456%
2	5.081	506	509	521	rVB	267559	305858	7.55%	0.993%
3	5.481	573	577	580	rBV	1889637	1690453	41.71%	5.487%
4	6.486	743	748	753	rBV	1282322	1111379	27.42%	3.608%
5	6.633	768	773	776	rBV	3005149	2903653	71.64%	9.426%
6	6.863	808	812	816	rBV	1006438	802147	19.79%	2.604%
7	7.022	832	839	842	rBV	2953216	2689513	66.36%	8.730%
8	7.427	902	908	911	rBV	2079909	2312983	57.07%	7.508%
9	7.510	916	922	925	rVV	134895	128614	3.17%	0.417%
10	8.145	1025	1030	1033	rBV	1362217	1124564	27.75%	3.650%
11	8.222	1036	1043	1045	rBV	201216	207230	5.11%	0.673%
12	8.316	1057	1059	1061	rVB	63899	45751	1.13%	0.149%
13	8.810	1140	1143	1149	rVB	144424	116125	2.87%	0.377%
14	8.874	1149	1154	1156	rBV	55873	50793	1.25%	0.165%
15	9.221	1207	1213	1216	rVB	3975132	4053144	100.00%	13.157%
16	9.610	1275	1279	1282	rVB	266504	203034	5.01%	0.659%
17	9.674	1286	1290	1295	rBV	131916	132948	3.28%	0.432%
18	9.904	1322	1329	1332	rBV	1286165	1285399	31.71%	4.173%
19	10.057	1350	1355	1358	rBV	179797	143035	3.53%	0.464%
20	10.216	1378	1382	1387	rVB	52749	48137	1.19%	0.156%
21	10.316	1393	1399	1403	rBV	154458	170161	4.20%	0.552%
22	10.439	1414	1420	1427	rVB3	73369	100971	2.49%	0.328%
23	10.498	1427	1430	1431	rBV	72288	70306	1.73%	0.228%
24	10.510	1431	1432	1434	rVV	97203	91790	2.26%	0.298%
25	10.527	1434	1435	1439	rVV2	133257	134790	3.33%	0.438%
26	10.557	1439	1440	1446	rVB	48403	40580	1.00%	0.132%
27	10.692	1454	1463	1466	rBV	2160720	2350940	58.00%	7.631%
28	10.792	1478	1480	1489	rVB3	44725	64866	1.60%	0.211%
29	10.874	1489	1494	1504	rBV2	120700	184252	4.55%	0.598%
30	10.998	1507	1515	1518	rBV5	36276	68530	1.69%	0.222%
31	11.339	1570	1573	1575	rBV	100556	80600	1.99%	0.262%
32	11.386	1578	1581	1585	rVV	1420009	1231428	30.38%	3.997%
33	11.433	1585	1589	1592	rVV4	59480	85576	2.11%	0.278%
34	11.504	1596	1601	1605	rBV4	31739	50522	1.25%	0.164%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.592	1612	1616	1618	rBV4	32131	43834	1.08%	0.142%
36	11.615	1618	1620	1622	rVB	54951	46525	1.15%	0.151%
37	11.762	1643	1645	1649	rVB2	57070	49675	1.23%	0.161%
38	11.862	1660	1662	1666	rVB	53089	45616	1.13%	0.148%
39	11.910	1666	1670	1673	rBV4	58496	72274	1.78%	0.235%
40	11.998	1681	1685	1689	rVB3	74517	90818	2.24%	0.295%
41	12.080	1696	1699	1703	rBV5	41780	44922	1.11%	0.146%
42	12.351	1742	1745	1747	rVB	71912	57284	1.41%	0.186%
43	12.598	1784	1787	1791	rBV	67027	65765	1.62%	0.213%
44	12.974	1846	1851	1854	rBV2	3344944	3675676	90.69%	11.932%
45	13.856	1998	2001	2008	rBV3	42006	50220	1.24%	0.163%
46	14.027	2026	2030	2033	rBV	983730	902718	22.27%	2.930%
47	15.498	2275	2280	2288	rVB	596909	727029	17.94%	2.360%
48	15.939	2350	2355	2362	rVB3	32113	52337	1.29%	0.170%
49	16.445	2437	2441	2447	rVB2	27606	44866	1.11%	0.146%

Sum of corrected areas: 30806223

LSC Report - Integrated Chromatogram

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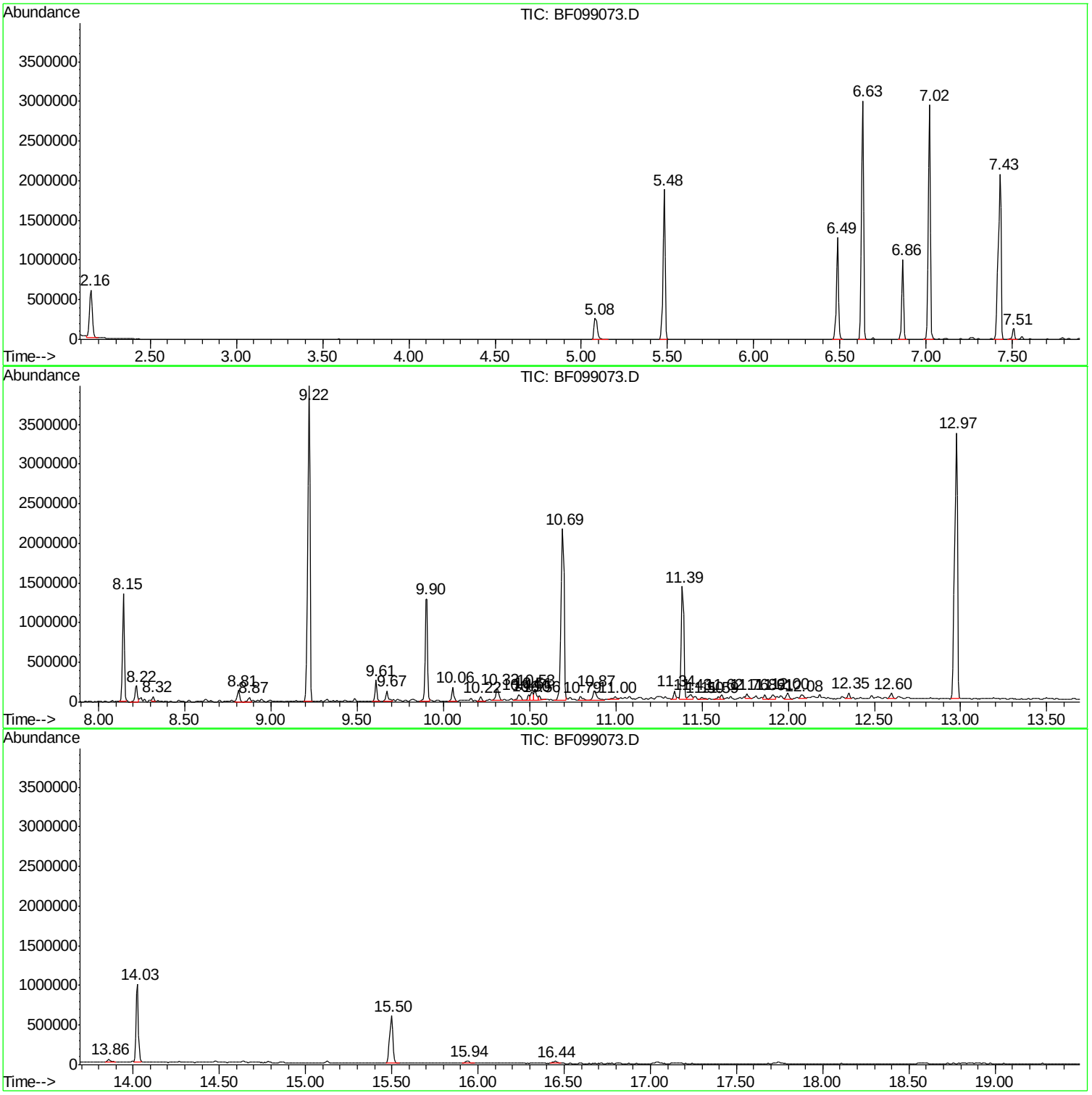
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF100417\
Data File : BF099073.D
Acq On : 4 Oct 2017 18:11
Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

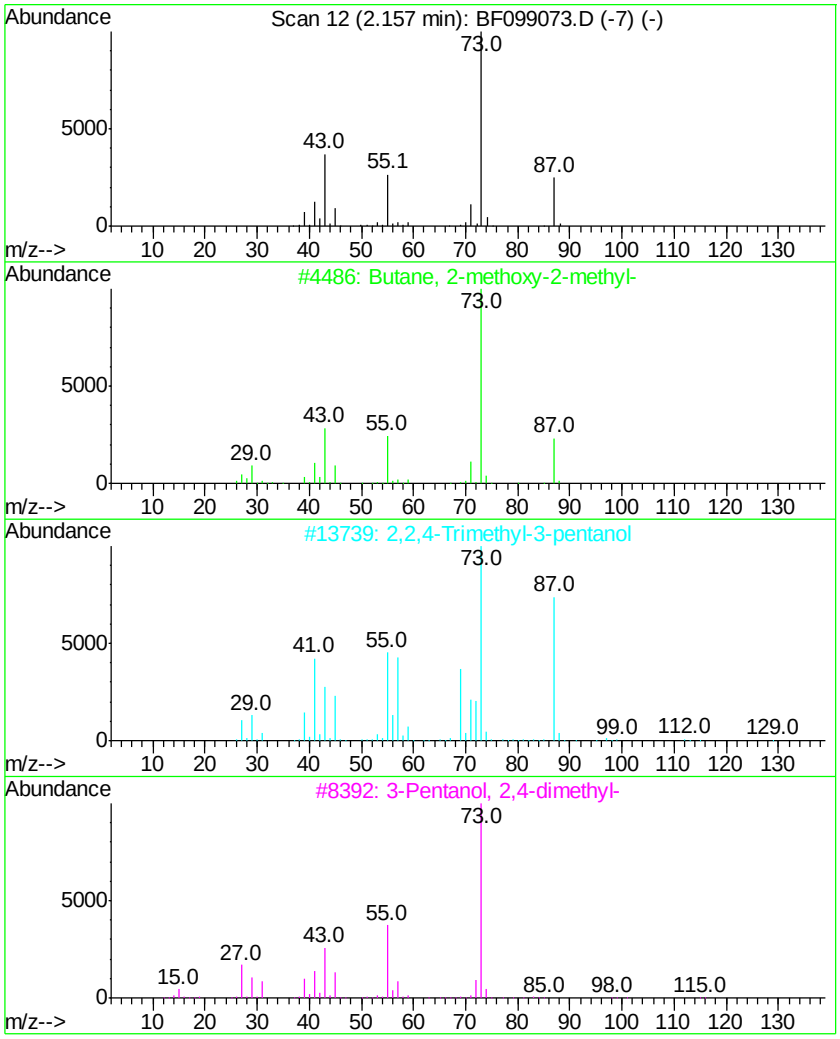
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

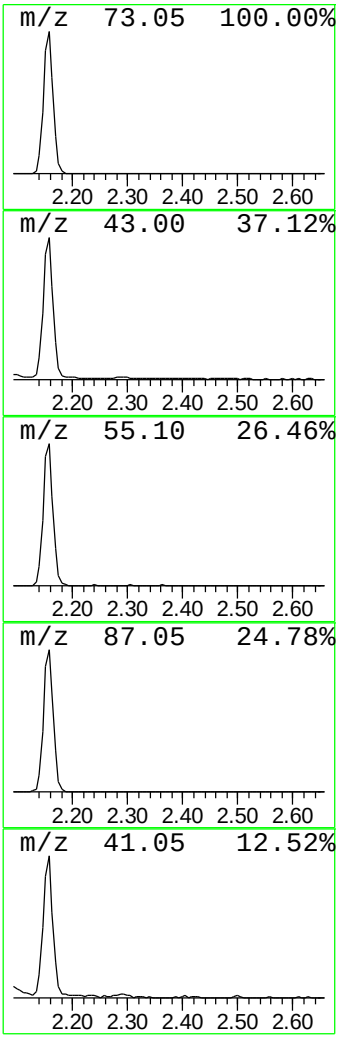
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	18.86 ng	756592	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
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Acq On : 4 Oct 2017 18:11
Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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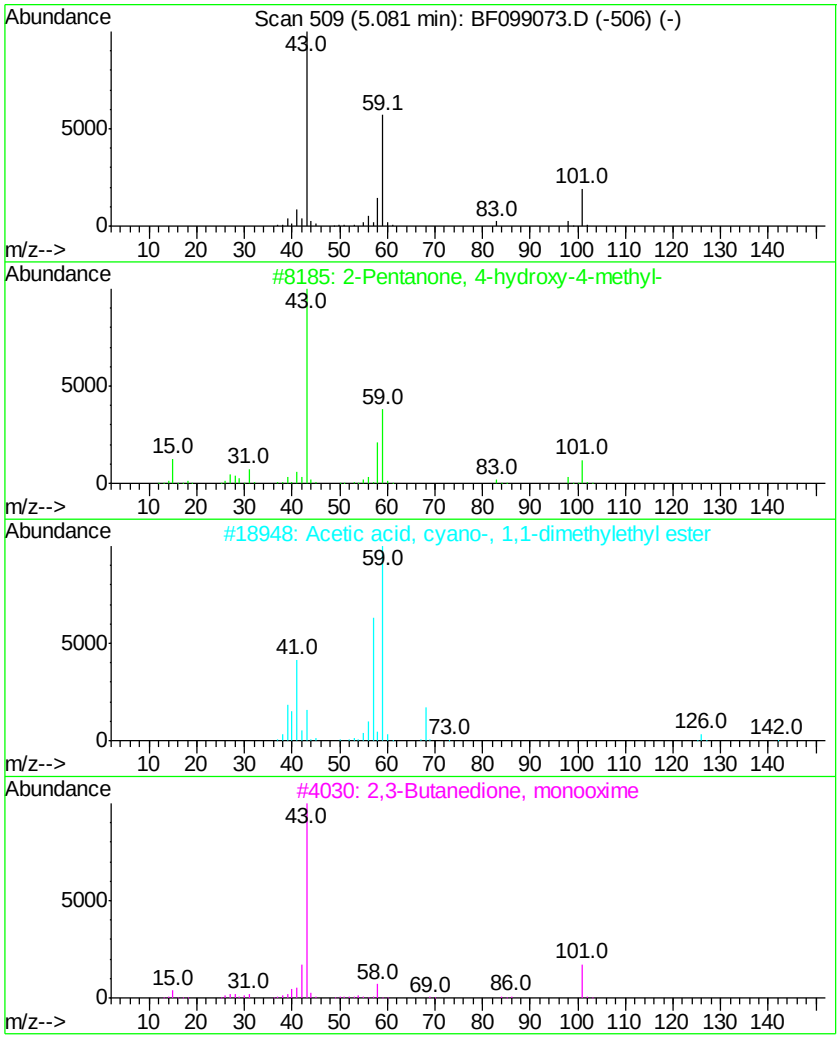
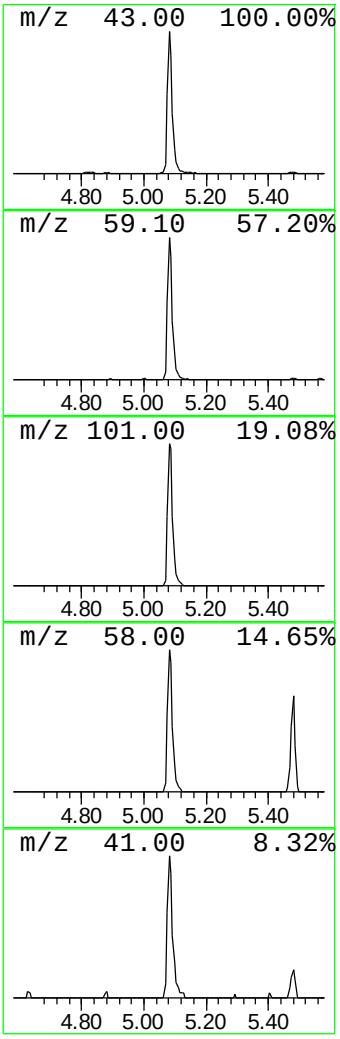
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	7.63 ng	305858	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099073.D
Acq On : 4 Oct 2017 18:11
Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

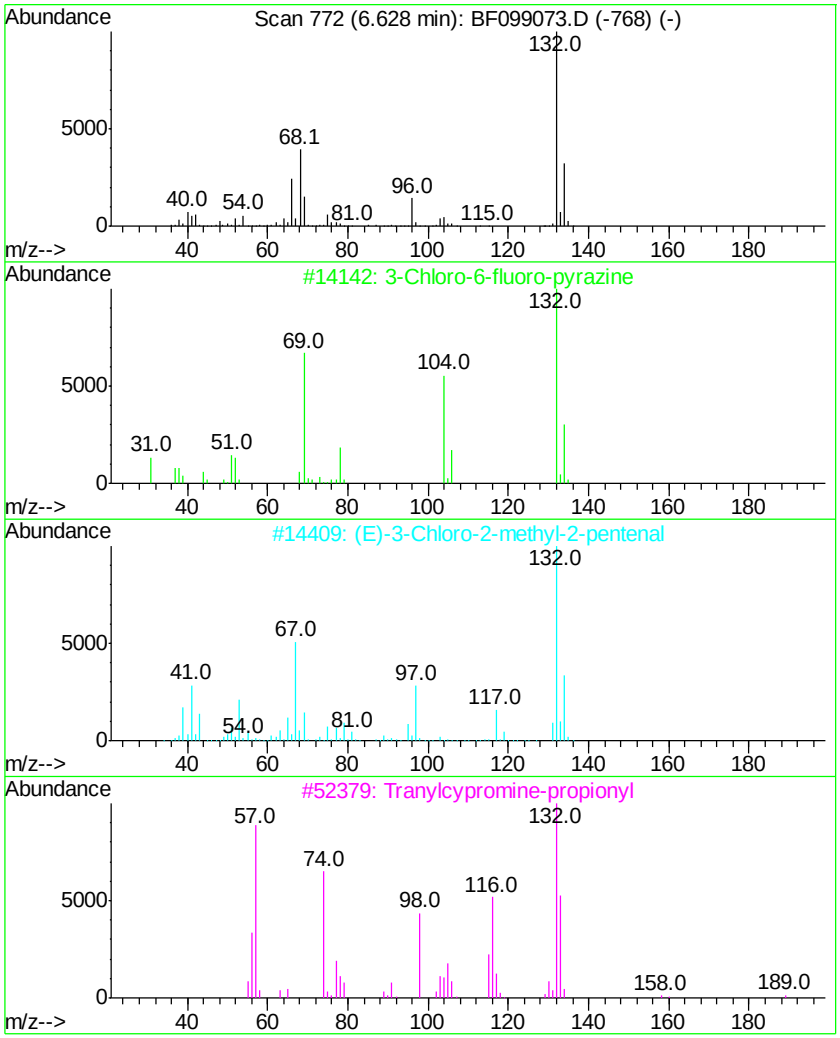
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

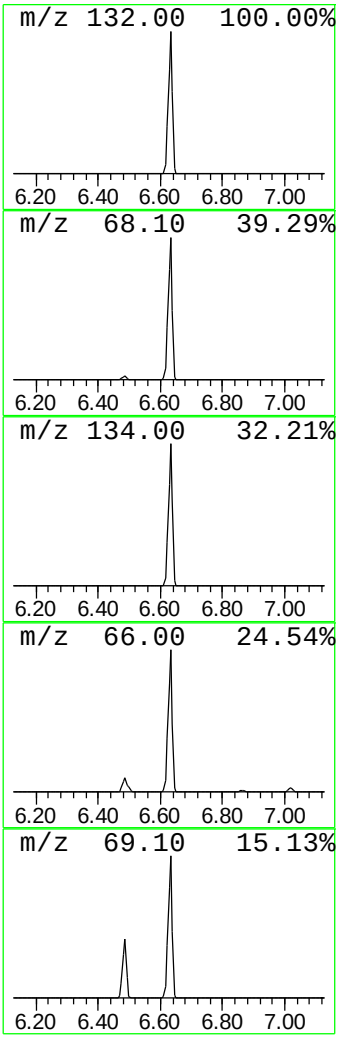
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	72.40 ng	2903650	1,4-Dichlorobenzene-d4	6.86

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

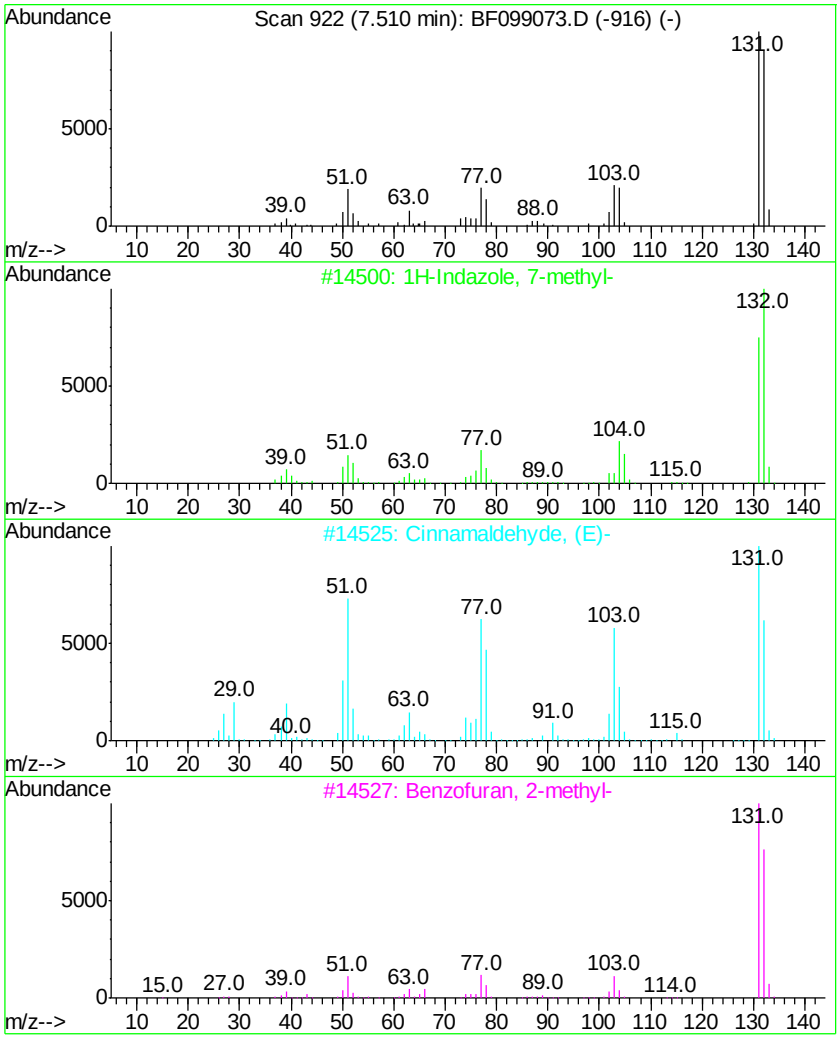
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

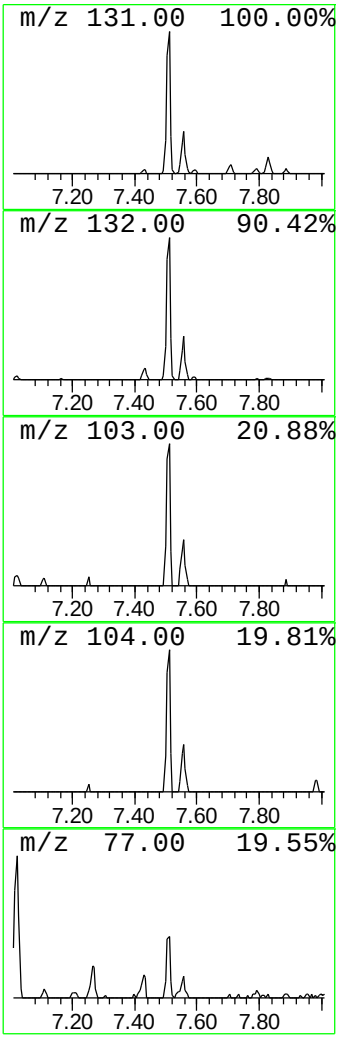
****

Peak Number 5 1H-Indazole, 7-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.51	2.29 ng	128614	Naphthalene-d8	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	90
2	Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	90
3	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	90
4	2-Propenal, 3-phenyl-	132	C9H8O	000104-55-2	87
5	3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	87





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Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

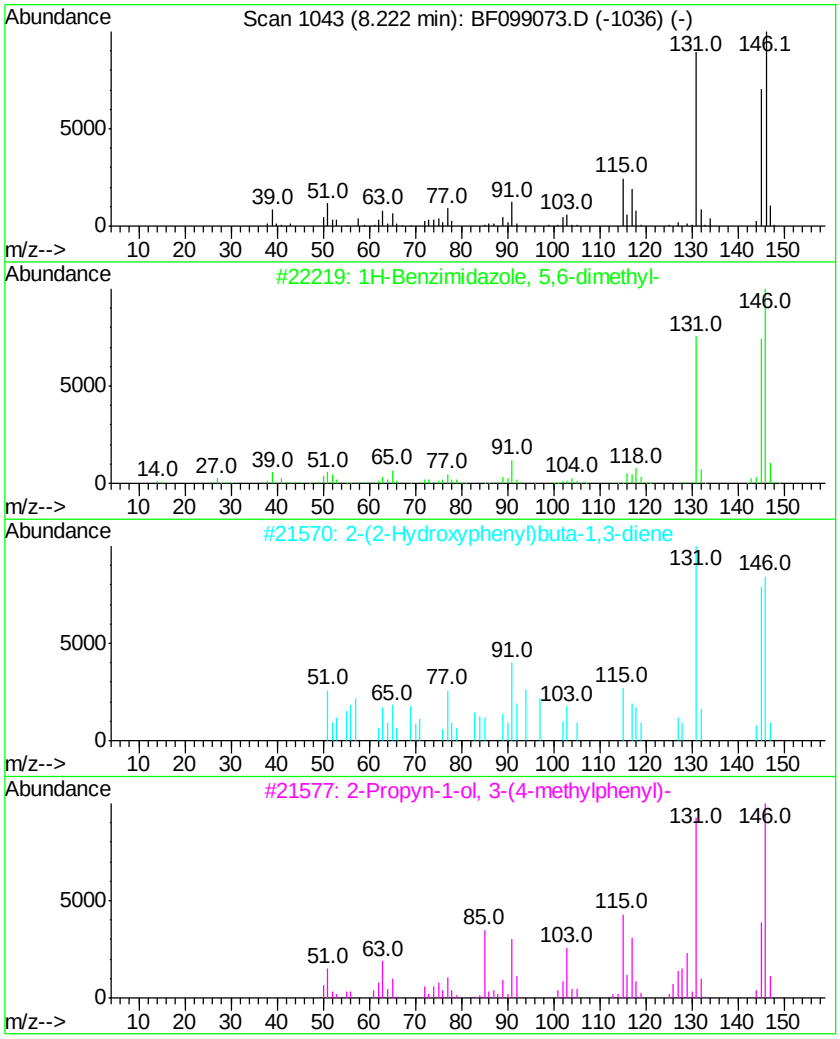
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

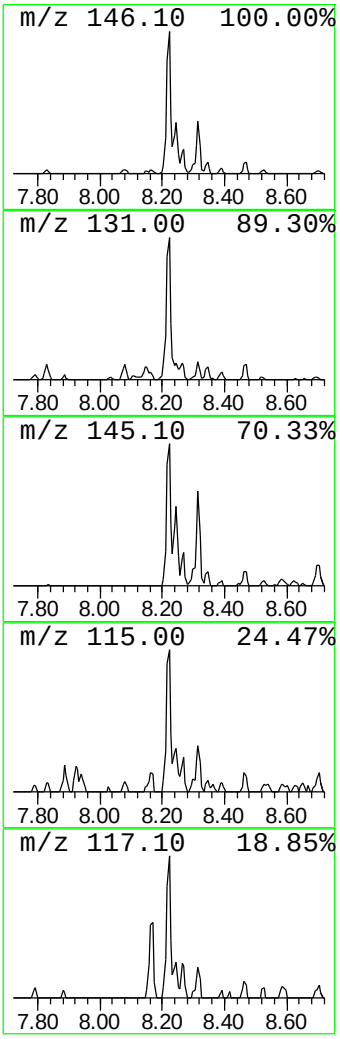
****

Peak Number 6 1H-Benzimidazole, 5,6-dimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.22	3.69 ng	207230	Naphthalene-d8	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	87
2	2-(2-Hydroxyphenyl)buta-1,3-diene	146	C10H10O	038865-47-3	86
3	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	83
4	1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	72
5	Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	72





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Sample : I5526-01
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Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

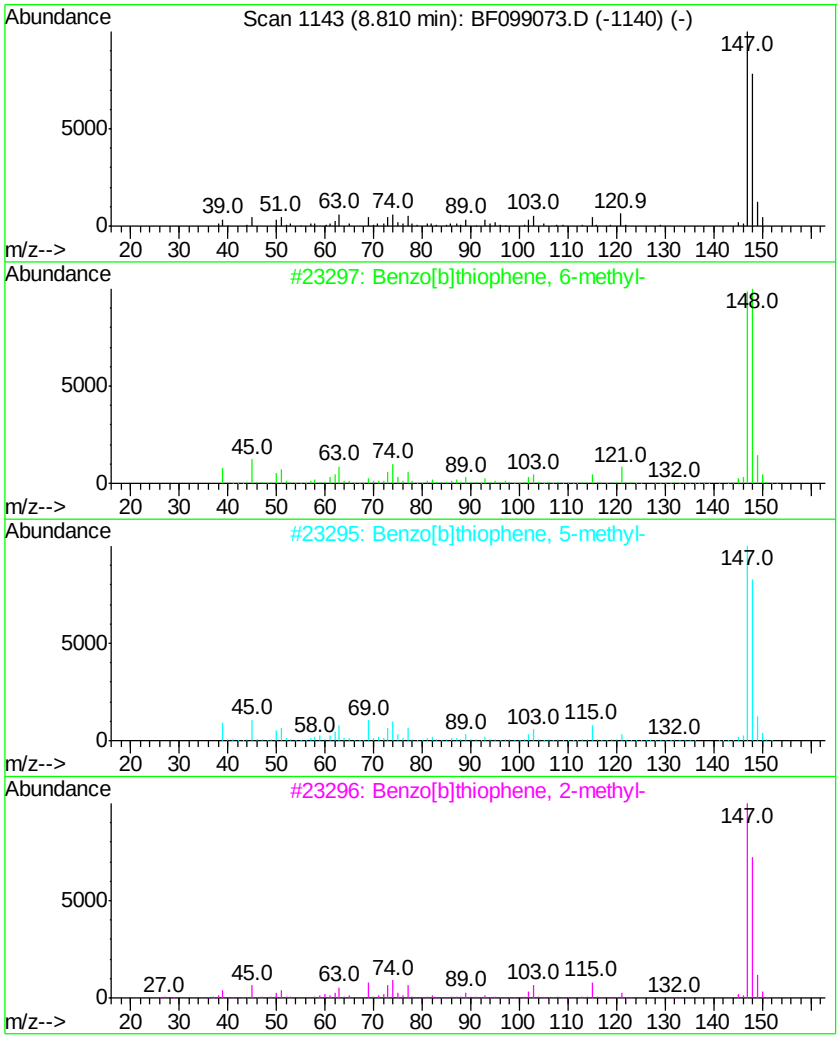
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

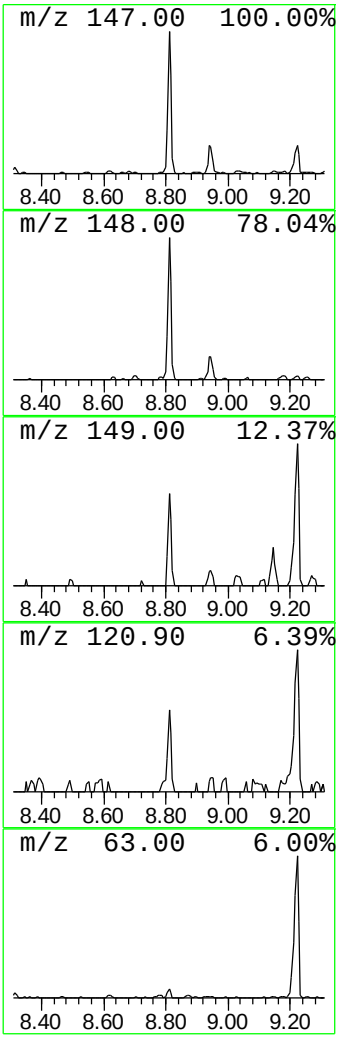
****

Peak Number 7 Benzo[b]thiophene, 6-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.81	2.07 ng	116125	Naphthalene-d8	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]thiophene, 6-methyl-	148	C9H8S	016587-47-6	91
2	Benzo[b]thiophene, 5-methyl-	148	C9H8S	014315-14-1	91
3	Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	91
4	Benzo[b]thiophene, 4-methyl-	148	C9H8S	014315-11-8	91
5	3-Methylbenzothiophene	148	C9H8S	001455-18-1	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
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Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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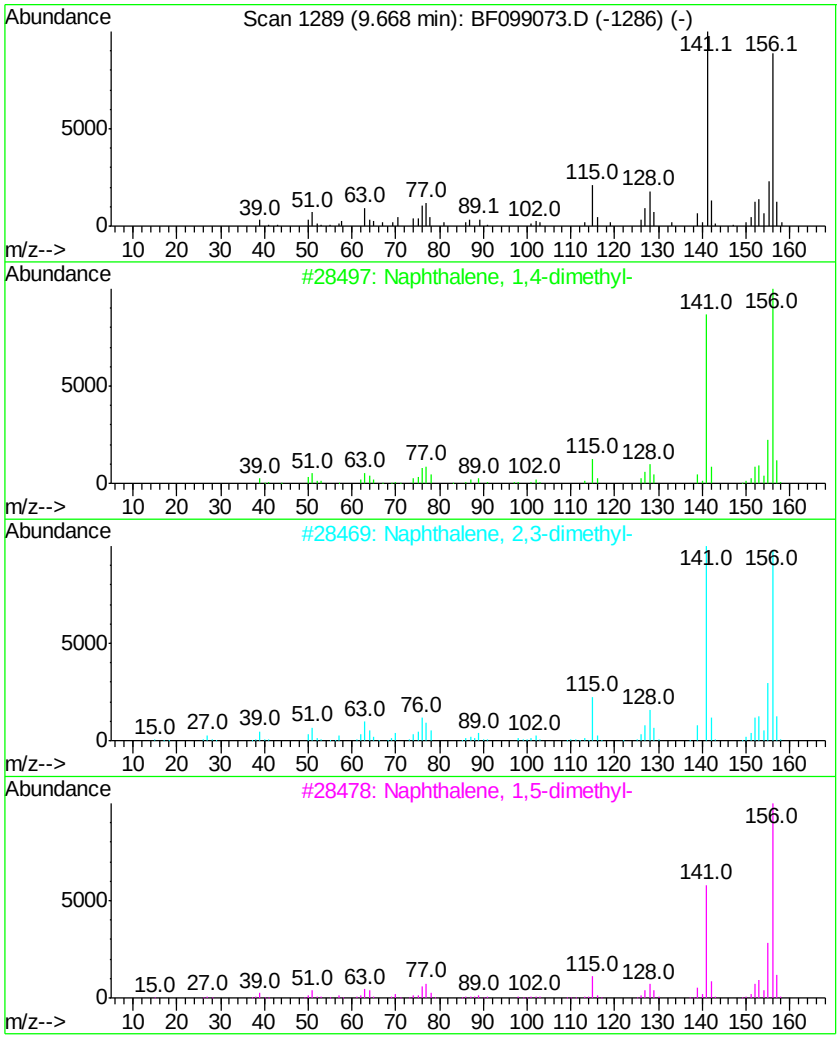
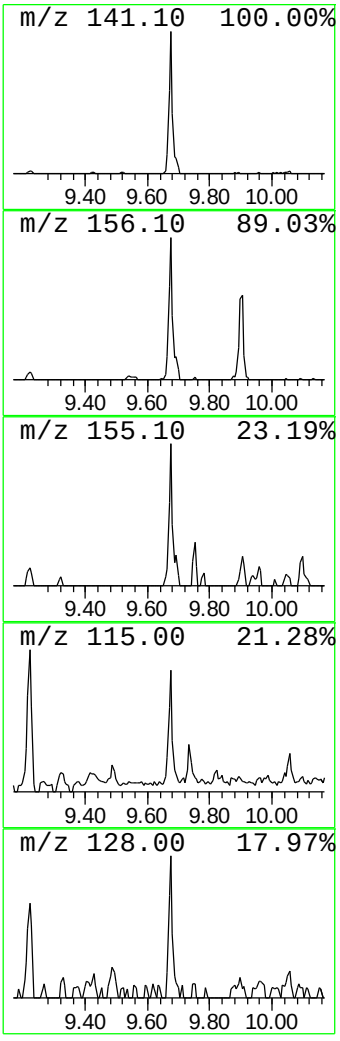
Peak Number 8 Naphthalene, 1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.67	2.07 ng	132948	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
3	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96





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Sample : I5526-01
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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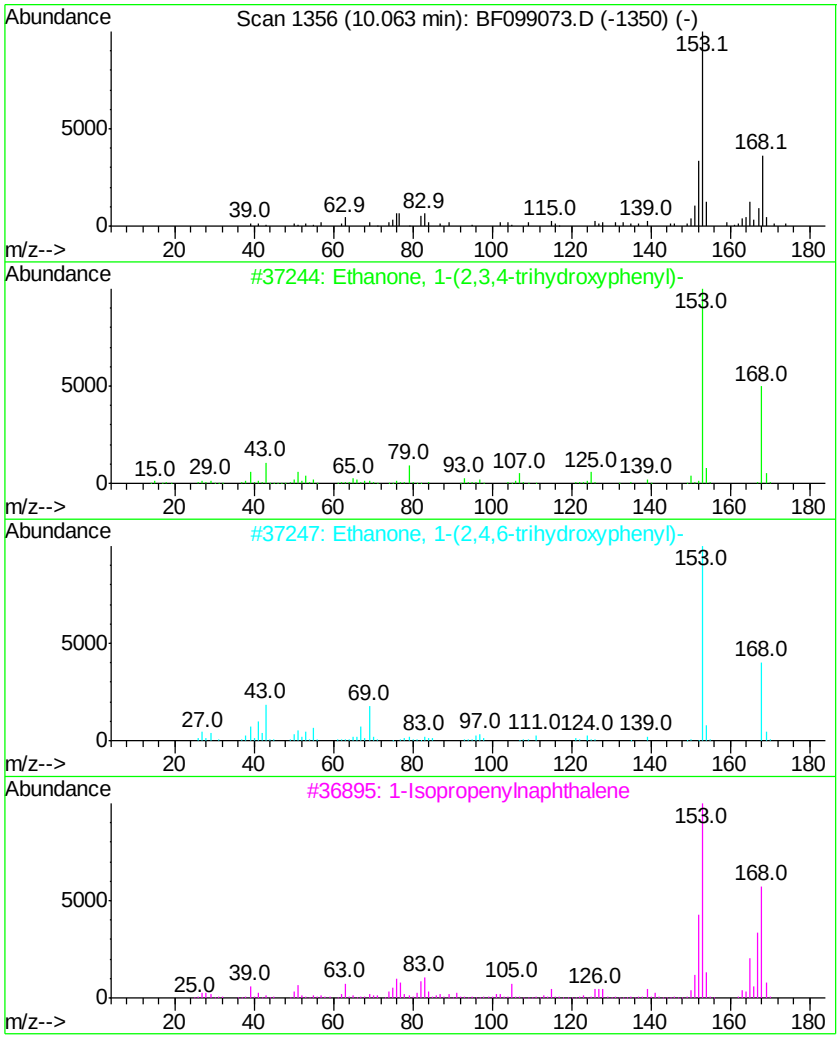
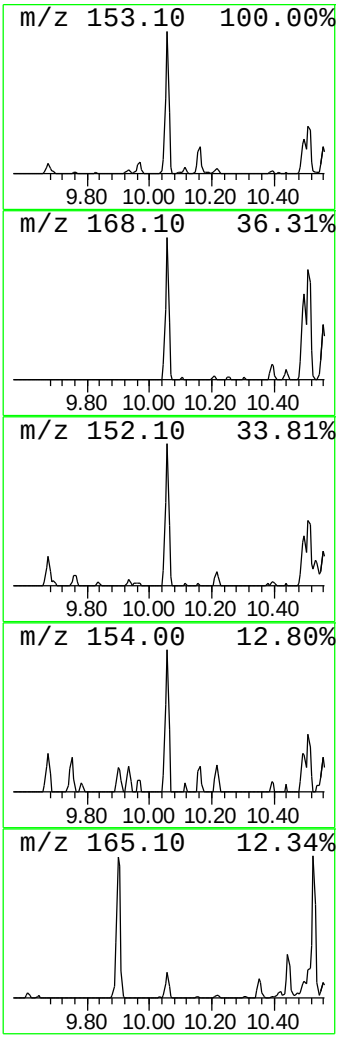
Peak Number 9 Ethanone, 1-(2,3,4-trihydro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.06	2.23 ng	143035	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(2,3,4-trihydroxyphe...	168	C8H8O4	000528-21-2	53
2	Ethanone, 1-(2,4,6-trihydroxyphe...	168	C8H8O4	000480-66-0	53
3	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	52
4	2,4(1H,3H)-Pyrimidinedione, 5-(1...	168	C8H12N2O2	017432-97-2	42
5	Thieno[2,3-b]thiophene, 2-ethyl-	168	C8H8S2	005912-01-6	42





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Acq On : 4 Oct 2017 18:11
Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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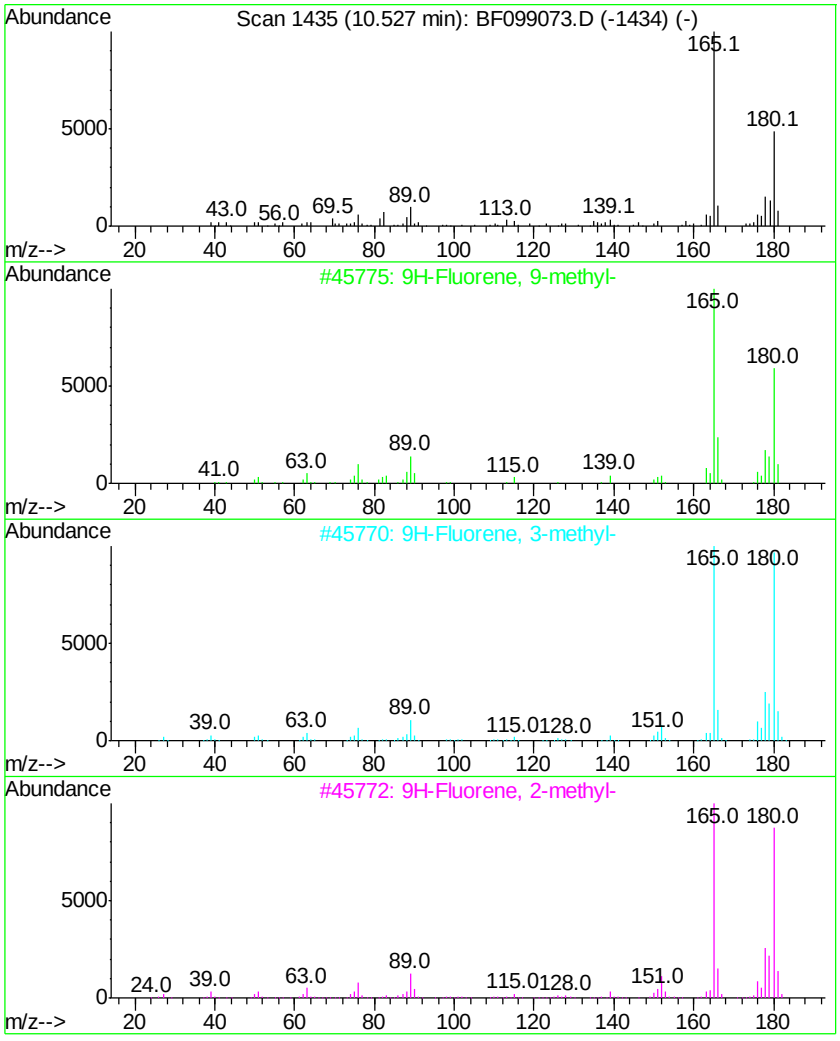
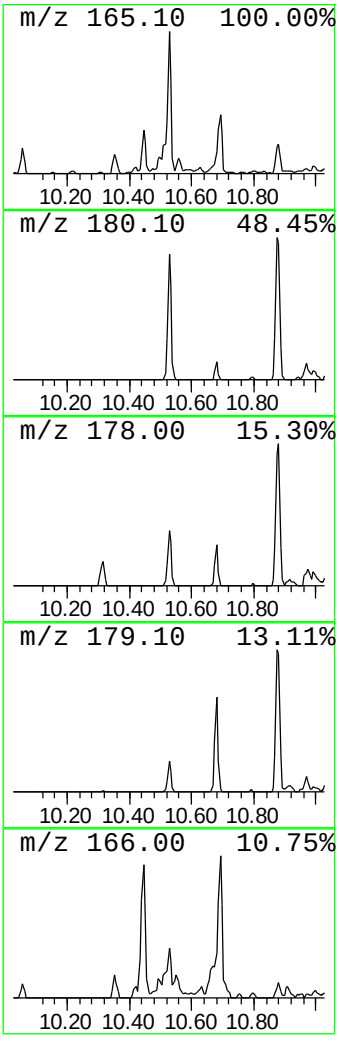
Peak Number 10 9H-Fluorene, 9-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	2.10 ng	134790	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9-methyl-	180	C14H12	002523-37-7	87
2	9H-Fluorene, 3-methyl-	180	C14H12	002523-39-9	87
3	9H-Fluorene, 2-methyl-	180	C14H12	001430-97-3	87
4	Thiazolo[5,4-d]pyrimidine, 5-(et...	180	C7H8N4S	019835-21-3	64
5	Borane, methyldiphenyl-	180	C13H13B	059073-99-3	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100417\
Data File : BF099073.D
Acq On : 4 Oct 2017 18:11
Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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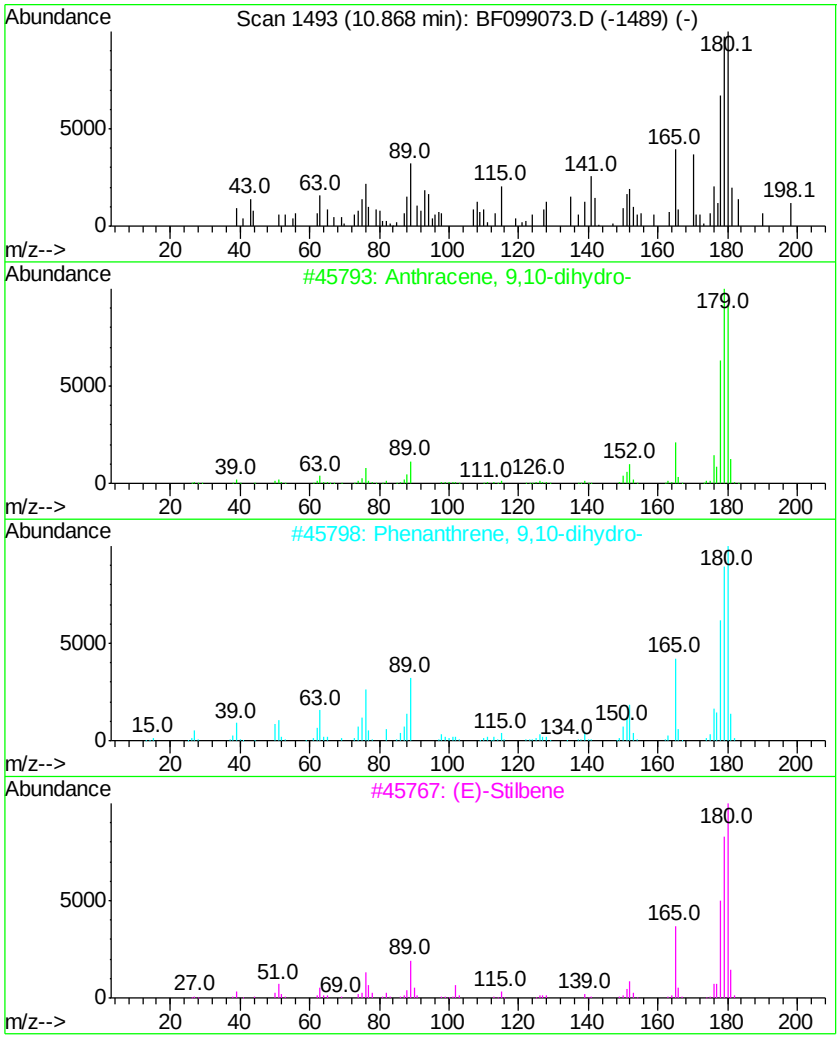
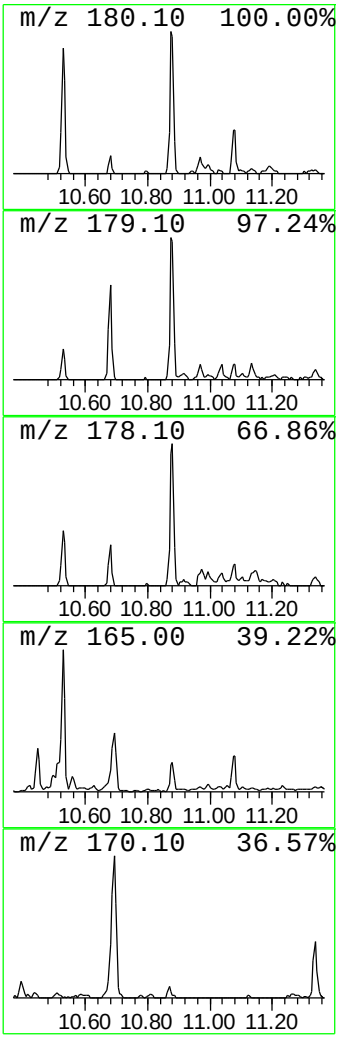
Peak Number 11 Anthracene, 9,10-dihydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.99 ng	184252	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9,10-dihydro-	180	C14H12	000613-31-0	95
2	Phenanthrene, 9,10-dihydro-	180	C14H12	000776-35-2	93
3	(E)-Stilbene	180	C14H12	000103-30-0	90
4	Phenanthrene, 1,2-dihydro-	180	C14H12	056179-83-0	90
5	cis-Stilbene	180	C14H12	000645-49-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100417\
Data File : BF099073.D
Acq On : 4 Oct 2017 18:11
Operator : SJ/JU
Sample : I5526-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : QNWP8-MW30S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.16	18.9	ng	756592	1	6.86	802147	20.0
2-Pentanone, 4-hy...	5.08	7.6	ng	305858	1	6.86	802147	20.0
unknown6.63	6.63	72.4	ng	2903650	1	6.86	802147	20.0
1H-Indazole, 7-me...	7.51	2.3	ng	128614	2	8.15	1124560	20.0
1H-Benzimidazole,...	8.22	3.7	ng	207230	2	8.15	1124560	20.0
Benzo[b]thiophene...	8.81	2.1	ng	116125	2	8.15	1124560	20.0
Naphthalene, 1,4-...	9.67	2.1	ng	132948	3	9.90	1285400	20.0
Ethanone, 1-(2,3,...	10.06	2.2	ng	143035	3	9.90	1285400	20.0
9H-Fluorene, 9-me...	10.53	2.1	ng	134790	3	9.90	1285400	20.0
Anthracene, 9,10-...	10.87	3.0	ng	184252	4	11.39	1231430	20.0