LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF073018\
Data File : BF107847.D
Acq On : 31 Jul 2018 12:49
Operator : JU/SJ
Sample : J4221-08
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ECMW-01

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-BF073018.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	5.195	482	486	503	rBV	198568	275388	5.46%	0.746%
2	5.601	551	555	569	rBV	1220856	1928615	38.25%	5.227%
3	6.601	722	725	744	rBV	658994	1601106	31.75%	4.339%
4	6.737	744	748	763	rVV	3224967	4017921	79.68%	10.890%
5	6.837	763	765	771	rVB4	46994	71484	1.42%	0.194%
6	6.966	783	787	806	rVB	562906	1011705	20.06%	2.742%
7	7.119	809	813	837	rVB	3115897	3841270	76.18%	10.411%
8	7.472	868	873	879	rBV8	26677	53596	1.06%	0.145%
9	7.531	879	883	892	rBV	1909180	2708275	53.71%	7.340%
10	7.678	905	908	912	rVB2	70718	69656	1.38%	0.189%
11	7.719	912	915	920	rVB2	71449	90547	1.80%	0.245%
12	7.825	932	933	939	rVB4	51045	56456	1.12%	0.153%
13	7.907	939	947	951	rVB6	65918	129691	2.57%	0.351%
14	7.960	951	956	959	rBV3	63440	110637	2.19%	0.300%
15	8.242	1000	1004	1014	rBV	938569	1300770	25.80%	3.525%
16	8.313	1014	1016	1019	rVB3	42529	50428	1.00%	0.137%
17	8.483	1042	1045	1048	rBV4	77973	74688	1.48%	0.202%
18	8.519	1048	1051	1055	rVB4	50347	52365	1.04%	0.142%
19	8.613	1063	1067	1074	rVB6	59974	126427	2.51%	0.343%
20	8.707	1078	1083	1090	rVV8	94409	170342	3.38%	0.462%
21	8.766	1090	1093	1096	rVB3	34823	51755	1.03%	0.140%
22	8.842	1104	1106	1111	rVB5	55246	54549	1.08%	0.148%
23	8.907	1114	1117	1119	rBV3	47047	52820	1.05%	0.143%
24	9.001	1130	1133	1135	rBV2	70534	75611	1.50%	0.205%
25	9.083	1144	1147	1152	rVB5	96550	155631	3.09%	0.422%
26	9.160	1156	1160	1162	rBV5	85448	98995	1.96%	0.268%
27	9.272	1175	1179	1182	rBV4	85323	126060	2.50%	0.342%
28	9.319	1182	1187	1200	rBV	4143235	5042259	100.00%	13.666%
29	9.478	1211	1214	1218	rVB2	48847	57014	1.13%	0.155%
30	9.666	1243	1246	1247	rBV2	90201	90066	1.79%	0.244%
31	9.707	1251	1253	1258	rVV	356323	349459	6.93%	0.947%
32	9.754	1259	1261	1266	rVV5	111725	133665	2.65%	0.362%
33	9.801	1266	1269	1274	rVB3	89225	128120	2.54%	0.347%
34	9.901	1283	1286	1294	rVB8	91683	127411	2.53%	0.345%

LSC Area Percent Report

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Sample : J4221-08
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ECMW-01

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-BF073018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.001	1297	1303	1314	rBV2	1239683	1377527	27.32%	3.733%
36	10.201	1333	1337	1342	rVB	78533	97889	1.94%	0.265%
37	10.248	1342	1345	1347	rBV	50027	52315	1.04%	0.142%
38	10.289	1349	1352	1354	rVB2	59695	53218	1.06%	0.144%
39	10.372	1361	1366	1370	rBV2	209626	294349	5.84%	0.798%
40	10.442	1374	1378	1384	rVB6	58461	95845	1.90%	0.260%
41	10.672	1413	1417	1423	rBV9	30226	68018	1.35%	0.184%
42	10.736	1423	1428	1435	rVV	153986	280755	5.57%	0.761%
43	10.801	1435	1439	1460	rVB	2190606	2908450	57.68%	7.883%
44	11.501	1554	1558	1565	rBV	841604	1138499	22.58%	3.086%
45	12.001	1640	1643	1647	rBV	68888	85996	1.71%	0.233%
46	13.083	1822	1827	1846	rBV	3336551	4005080	79.43%	10.855%
47	14.154	2005	2009	2022	rBV	767927	1140939	22.63%	3.092%
48	15.689	2265	2270	2285	rVB	558086	1013071	20.09%	2.746%

Sum of corrected areas: 36896733

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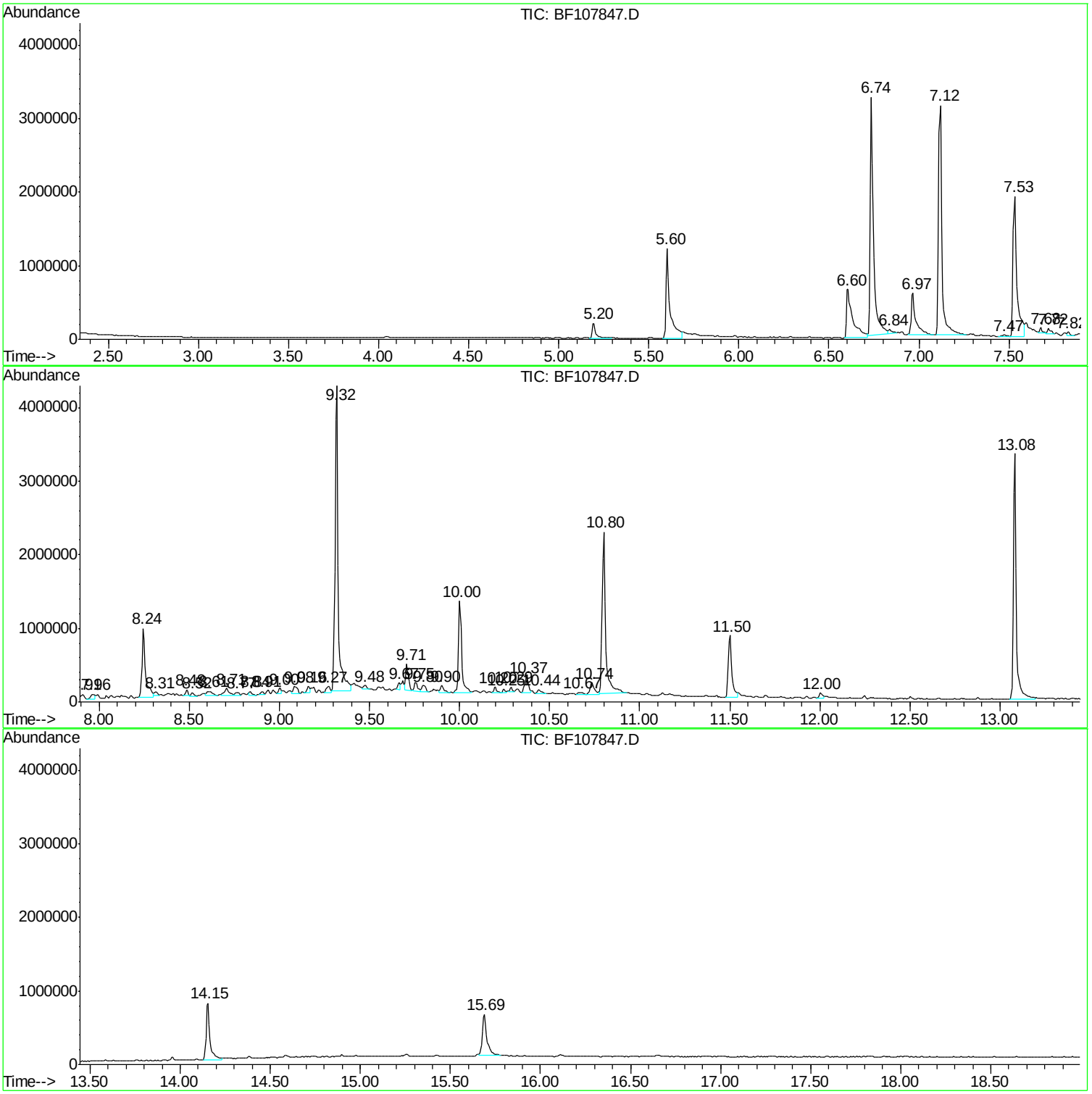
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ECMW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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

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Data File : BF107847.D
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Sample : J4221-08
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ECMW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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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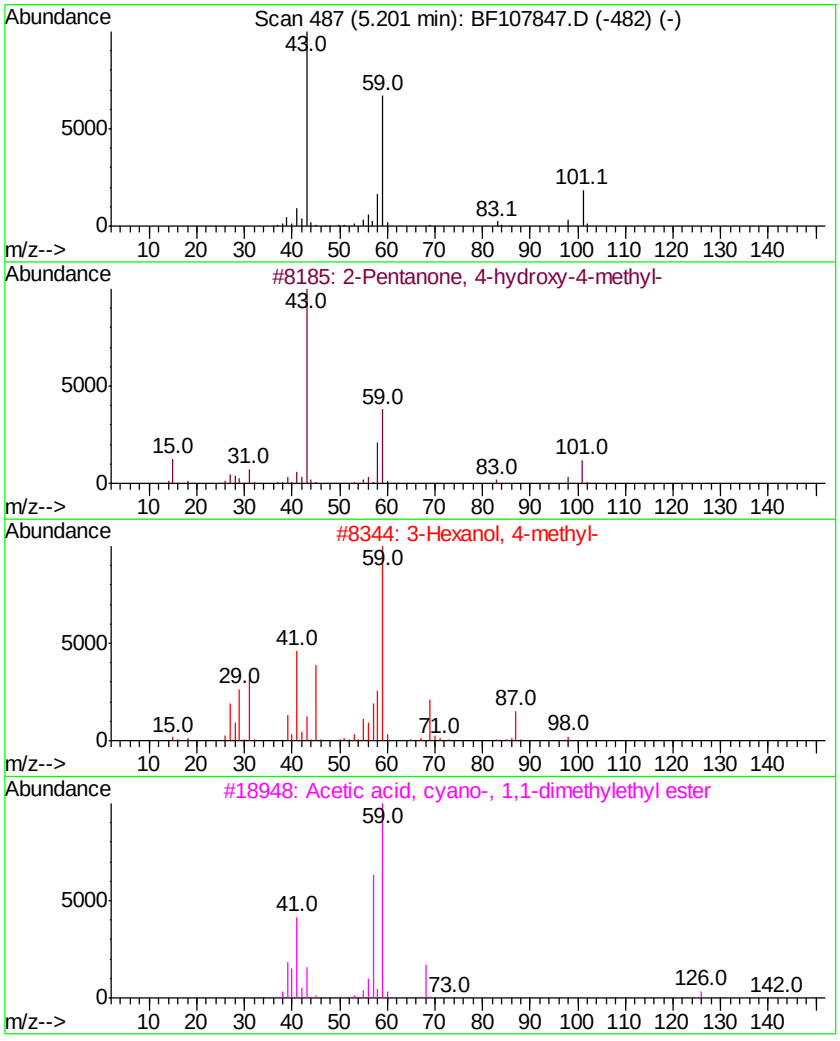
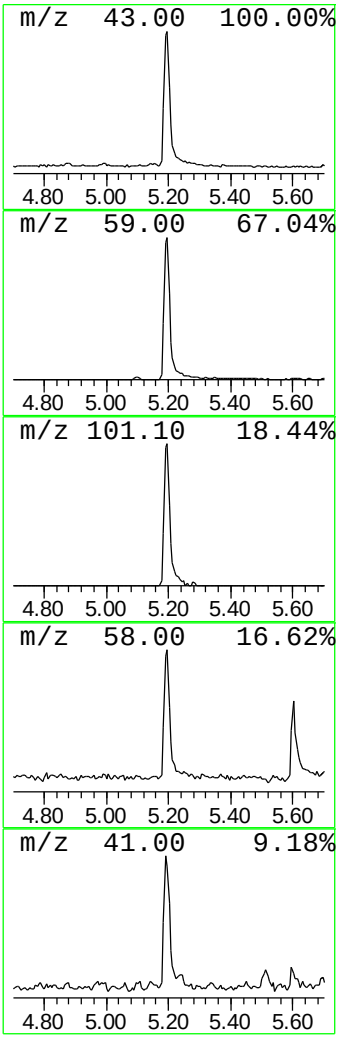
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.44 ng	275388	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	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Guanidine	59	CH5N3	000113-00-8	9





Library Search Compound Report

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Data File : BF107847.D
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Operator : JU/SJ
Sample : J4221-08
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ECMW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

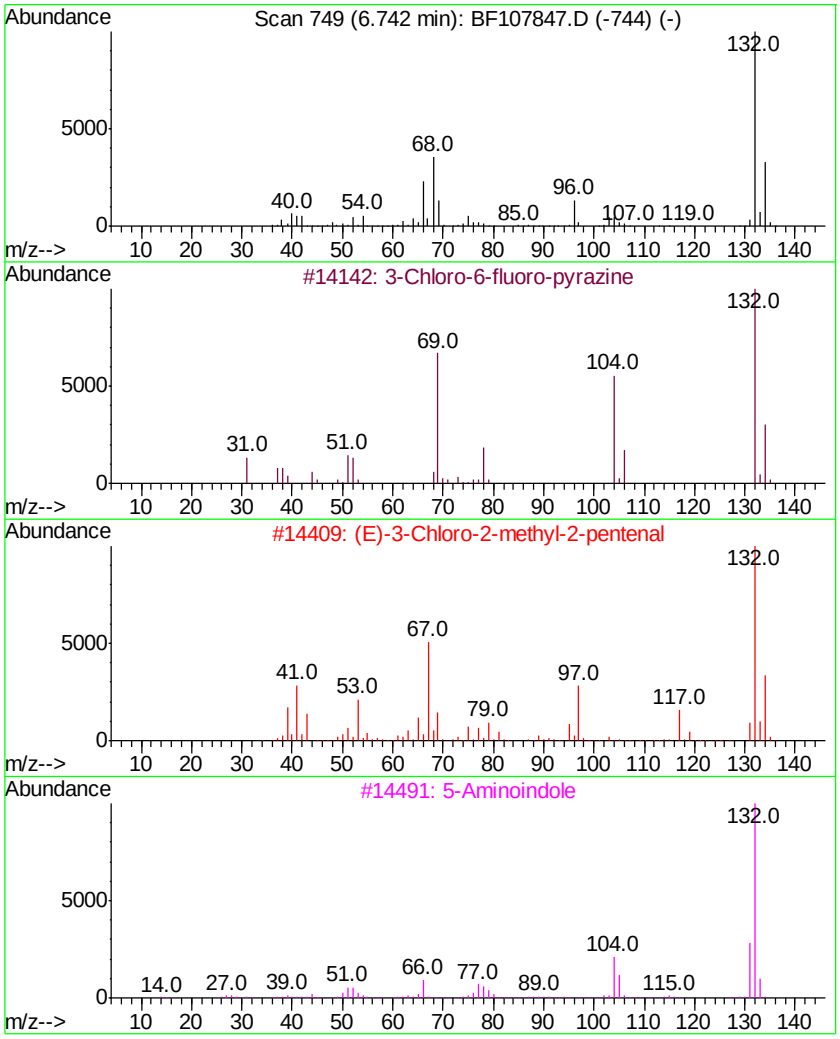
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

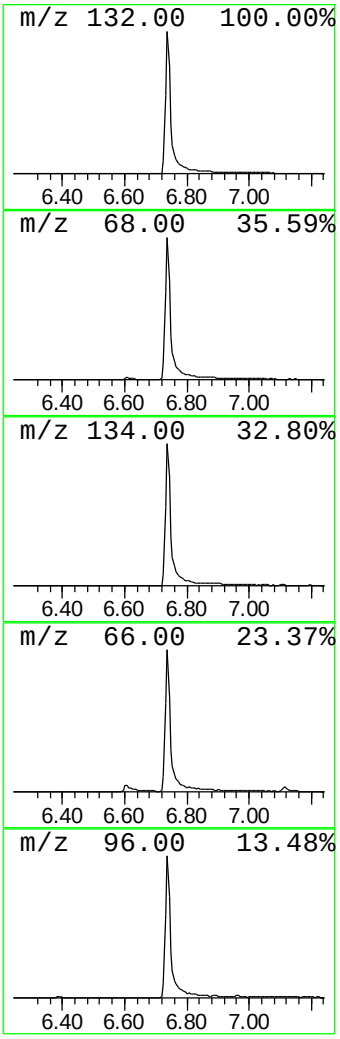
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	79.43 ng	4017920	1,4-Dichlorobenzene-d4	6.97

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Acq On : 31 Jul 2018 12:49
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Sample : J4221-08
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ECMW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

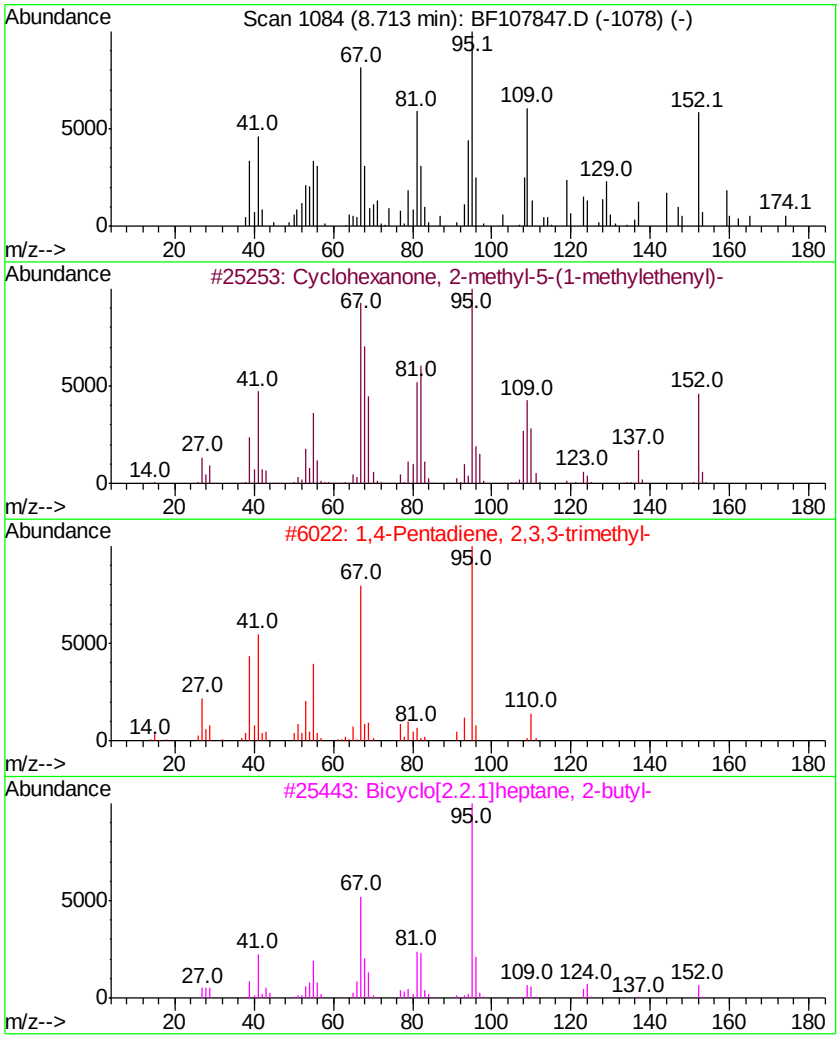
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

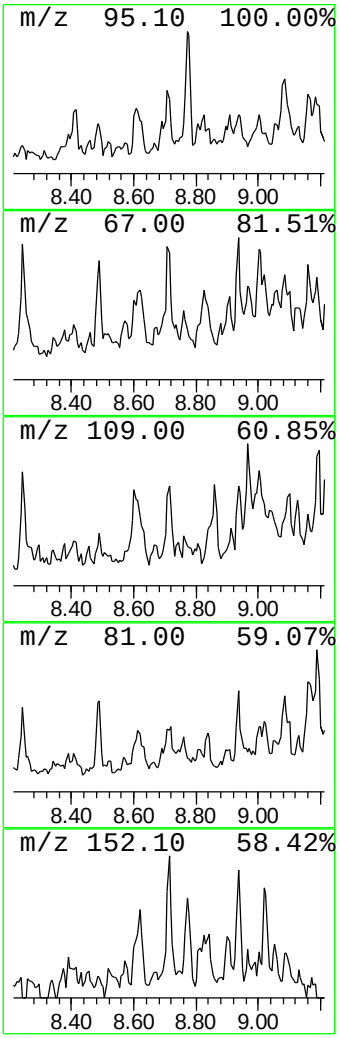
****

Peak Number 4 unknown8.71 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.71	2.62 ng	170342	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	49
2	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	42
3	Bicyclo[2.2.1]heptane, 2-butyl-	152	C11H20	061177-16-0	41
4	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38
5	2-Isopropylidene-5-methylhex-4-enal	152	C10H16O	003304-28-7	30





Library Search Compound Report

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Sample : J4221-08
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ECMW-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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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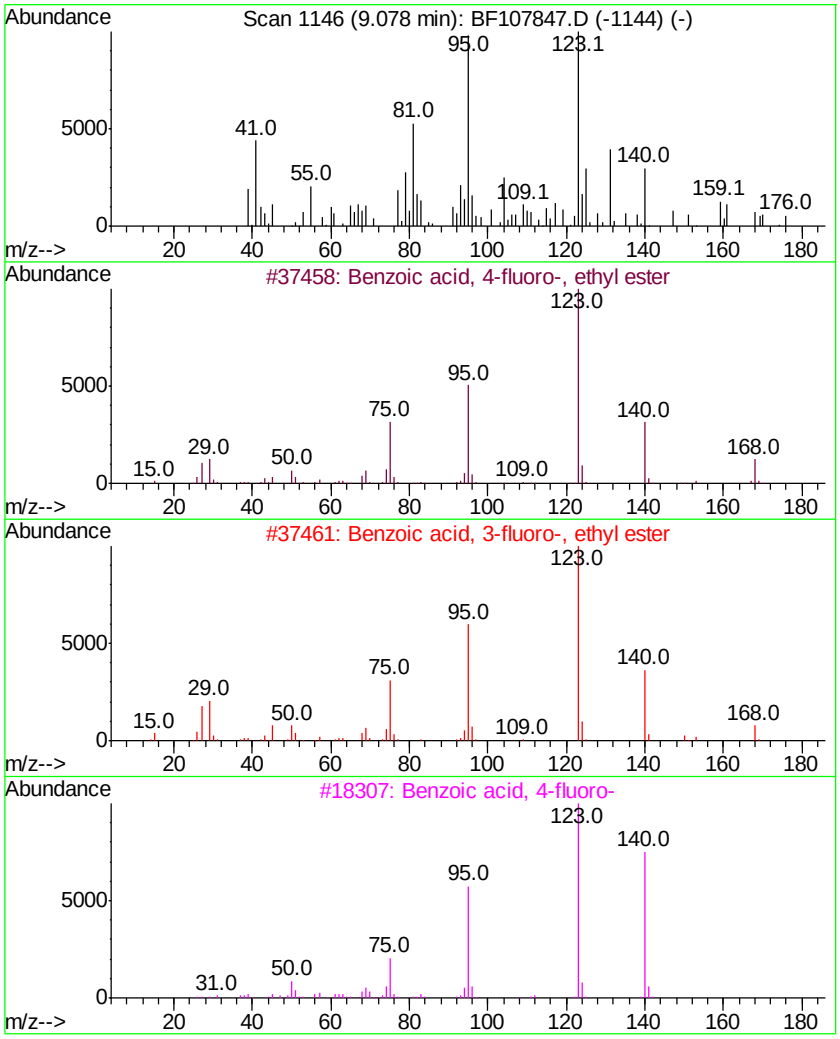
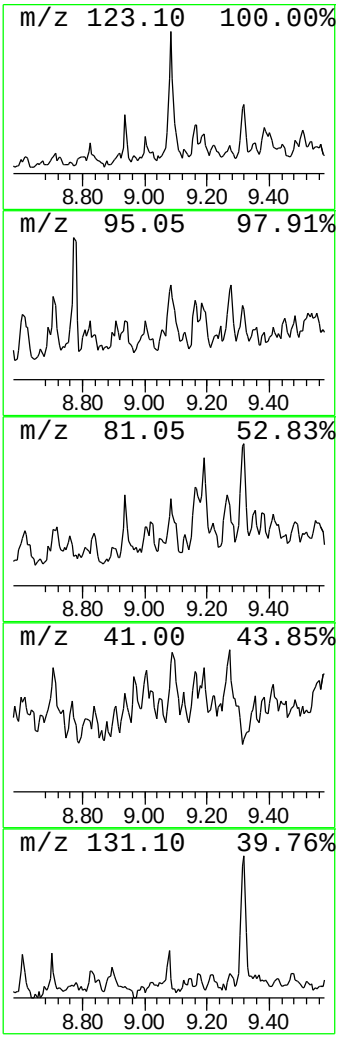
Peak Number 5 Benzoic acid, 4-fluoro-, et... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.08	2.39 ng	155631	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-fluoro-, ethyl e...	168	C9H9FO2	000451-46-7	68
2	Benzoic acid, 3-fluoro-, ethyl e...	168	C9H9FO2	000451-02-5	68
3	Benzoic acid, 4-fluoro-	140	C7H5FO2	000456-22-4	53
4	Benzoic acid, 2-fluoro-, ethyl e...	168	C9H9FO2	000443-26-5	52
5	Phorone	138	C9H14O	000504-20-1	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

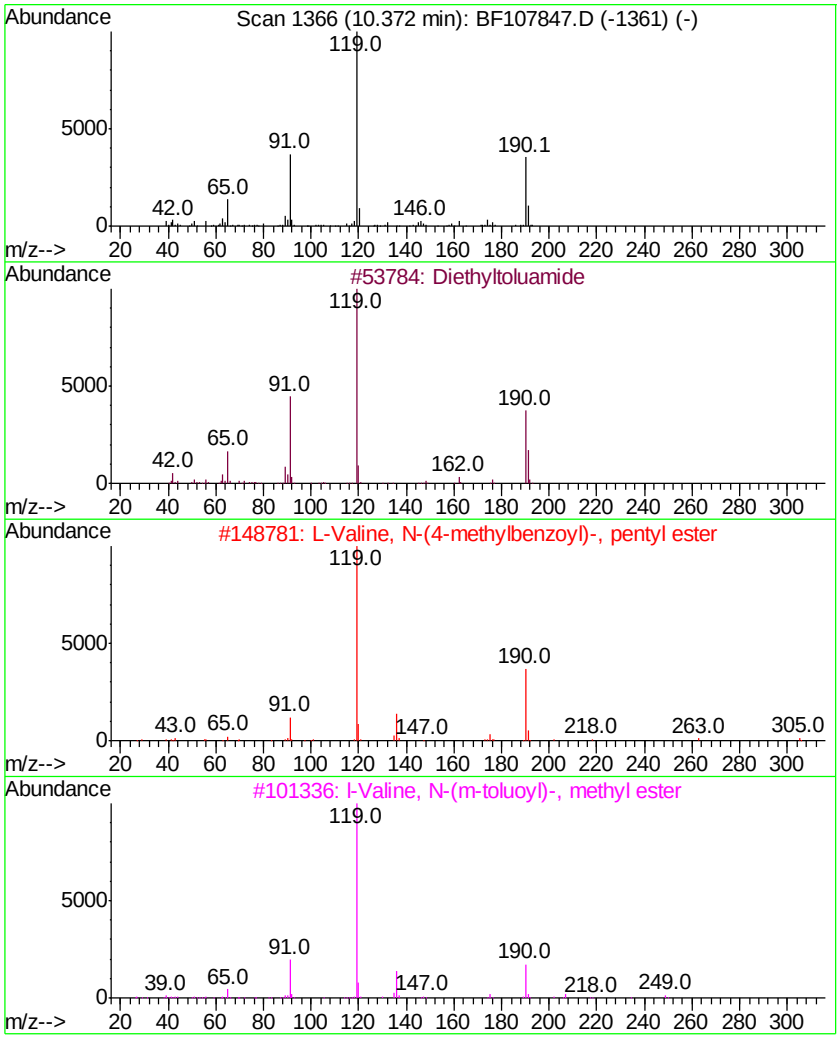
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

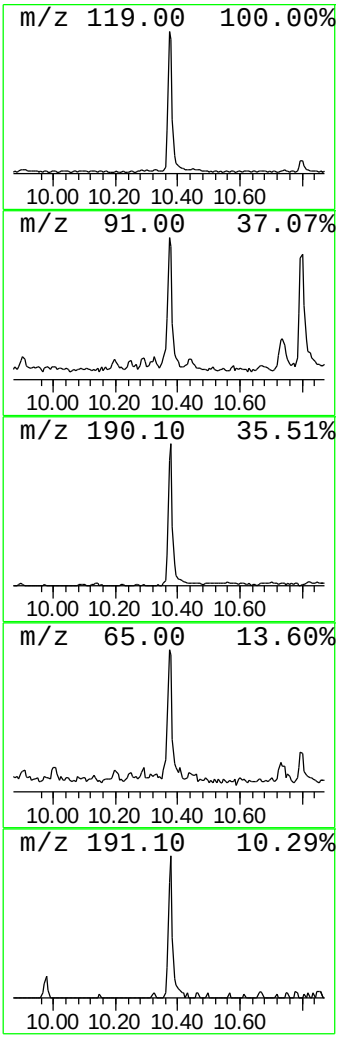
****

Peak Number 6 Diethyltoluamide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	4.27 ng	294349	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	87
2	L-Valine, N-(4-methylbenzoyl)-, ...	305	C18H27NO3	1000346-64-1	72
3	l-Valine, N-(m-toluoyl)-, methyl...	249	C14H19NO3	1000299-63-9	72
4	l-Valine, N-(p-toluoyl)-, methyl...	249	C14H19NO3	1000299-64-7	72
5	N-[1-(Dimethylamino)-2,2,2-trich...	308	C12H15Cl3N2O	300814-41-9	64





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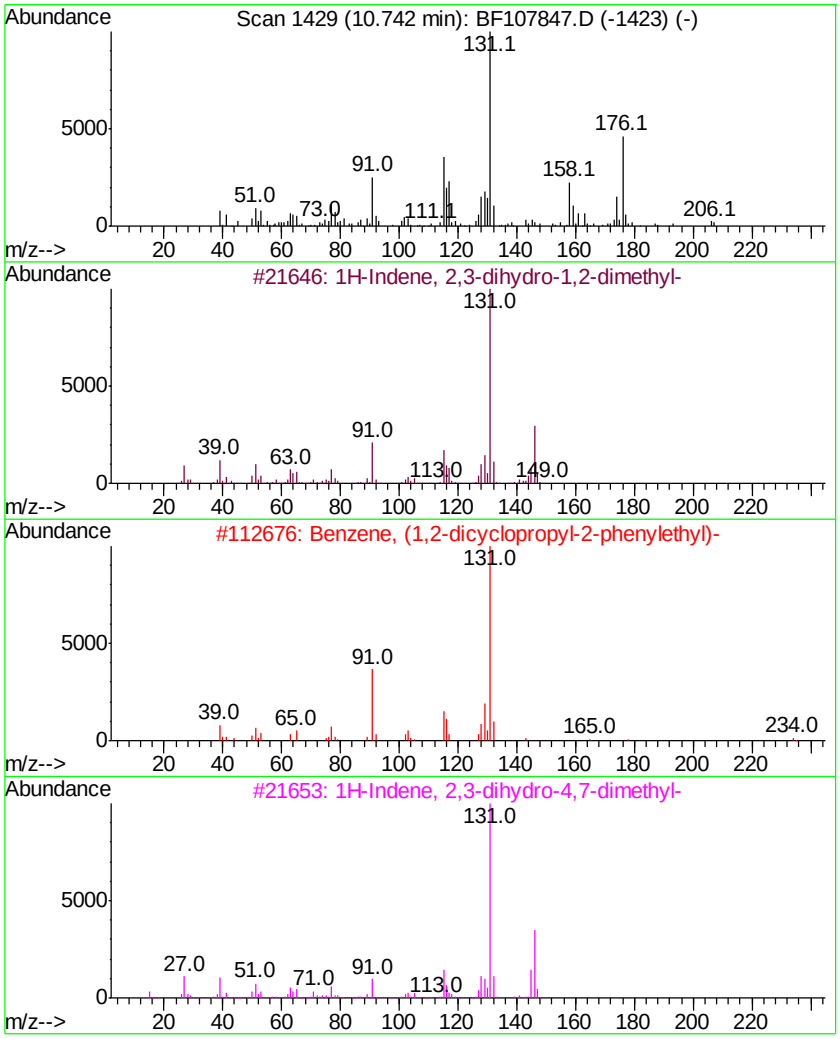
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

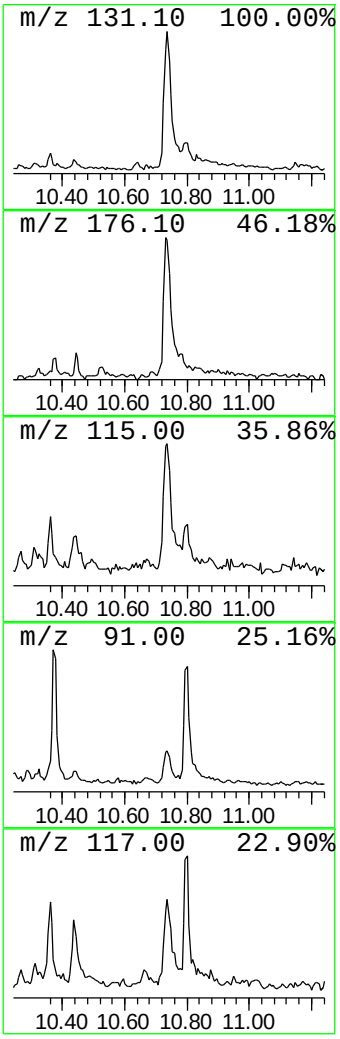
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	4.08 ng	280755	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	50
2	Benzene, (1,2-dicyclopropyl-2-ph...	262	C20H22	110330-90-0	47
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	47
4	Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	43
5	[2-(Hydroxy-phenyl-phosphinoyl)-...	316	C15H13N2O4P	300566-65-8	43





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.20	5.4	ng	275388	1	6.97	1011710	20.0
unknown6.74	6.74	79.4	ng	4017920	1	6.97	1011710	20.0
unknown8.71	8.71	2.6	ng	170342	2	8.24	1300770	20.0
Benzoic acid, 4-f...	9.08	2.4	ng	155631	2	8.24	1300770	20.0
Diethyltoluamide	10.37	4.3	ng	294349	3	10.00	1377530	20.0
1H-Indene, 2,3-di...	10.74	4.1	ng	280755	3	10.00	1377530	20.0