LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020724\
Data File : BF137330.D
Acq On : 07 Feb 2024 20:04
Operator : CG\JU
Sample : P1342-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317AP-GW-20240131-0

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-BF013024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137330.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.869	298	303	312	rBV	254688	354316	2.31%	0.559%
2	5.416	562	566	576	rBV	888068	812355	5.29%	1.282%
3	6.422	733	737	749	rBV	326671	473450	3.09%	0.747%
4	6.786	796	799	807	rBV	383920	322505	2.10%	0.509%
5	6.863	807	812	819	rBV	322453	406069	2.65%	0.641%
6	6.981	819	832	834	rBV	4800704	10900317	71.04%	17.208%
7	7.351	891	895	907	rBV	1216327	1298378	8.46%	2.050%
8	7.716	946	957	960	rBV	5311587	9995121	65.14%	15.779%
9	7.992	970	1004	1007	rBV2	937732	4681365	30.51%	7.390%
10	8.069	1014	1017	1019	rBV	601160	578218	3.77%	0.913%
11	8.780	1094	1138	1141	rBV	2226247	15343497	100.00%	24.222%
12	9.104	1188	1193	1197	rBV	3129269	3277364	21.36%	5.174%
13	9.151	1197	1201	1204	rVB	2204212	2135012	13.91%	3.370%
14	9.822	1297	1315	1317	rBV	1584929	4571306	29.79%	7.217%
15	9.892	1317	1327	1329	rBV	1387934	3363167	21.92%	5.309%
16	10.251	1383	1388	1405	rVB	525192	914998	5.96%	1.444%
17	10.616	1446	1450	1462	rBV	1175590	1152449	7.51%	1.819%
18	11.316	1565	1569	1585	rVB	408656	394166	2.57%	0.622%
19	12.910	1836	1840	1844	rBV	1829127	1713718	11.17%	2.705%
20	13.962	2016	2019	2029	rBV	372852	358301	2.34%	0.566%
21	15.445	2267	2271	2279	rBV	233718	298901	1.95%	0.472%

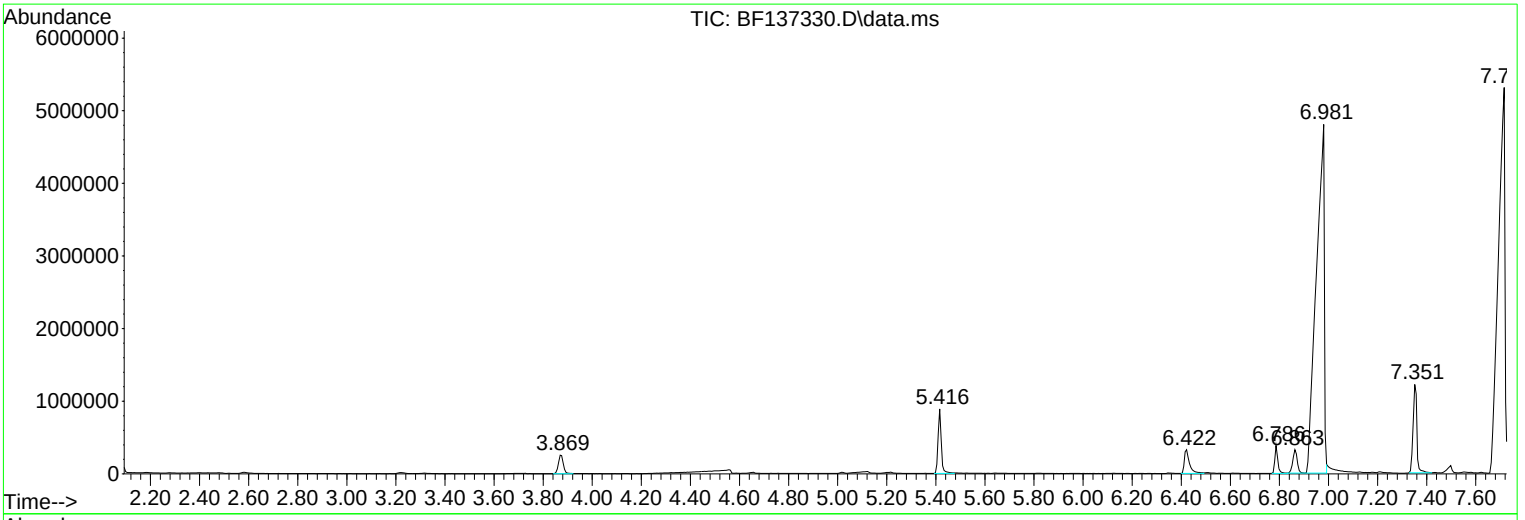
Sum of corrected areas: 63344973

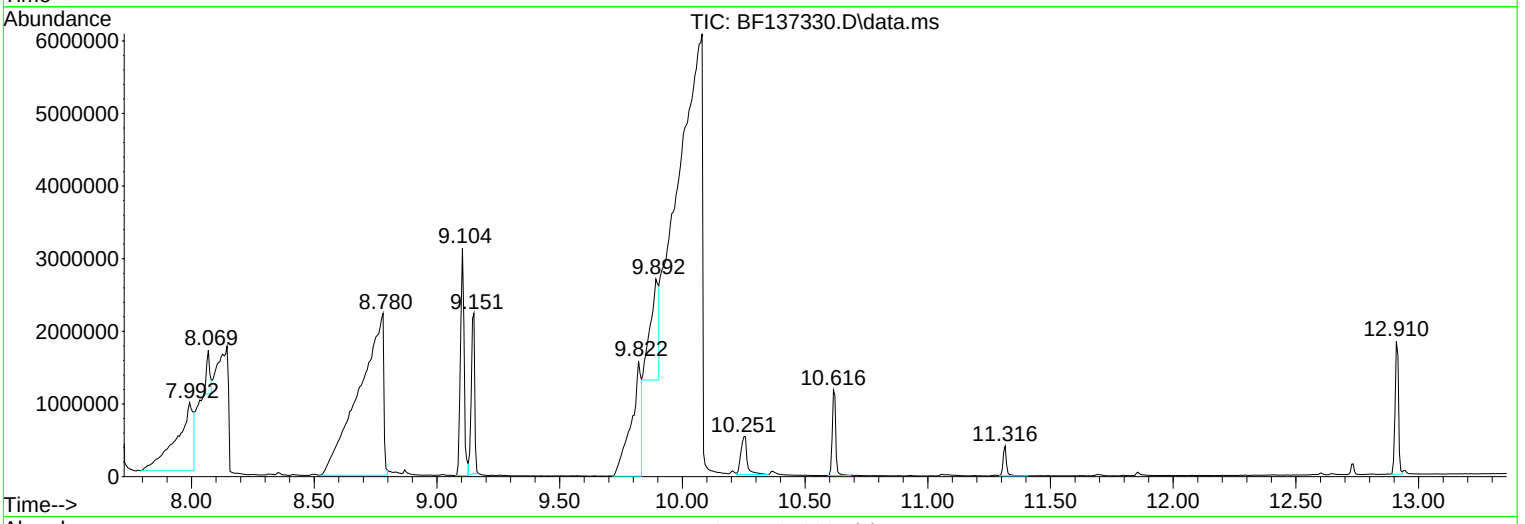
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020724\
Data File : BF137330.D
Acq On : 07 Feb 2024 20:04
Operator : CG\JU
Sample : P1342-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

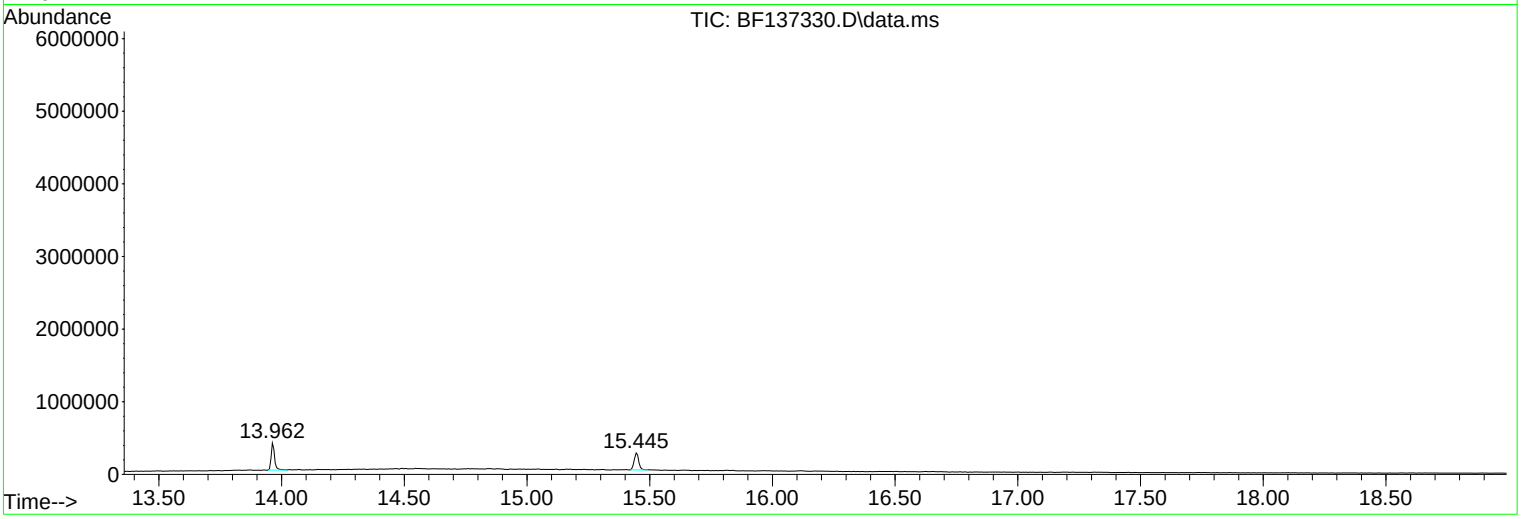
Instrument :
BNA_F
ClientSampleId :
MR-317AP-GW-20240131-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020724\
Data File : BF137330.D
Acq On : 07 Feb 2024 20:04
Operator : CG\JU
Sample : P1342-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317AP-GW-20240131-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

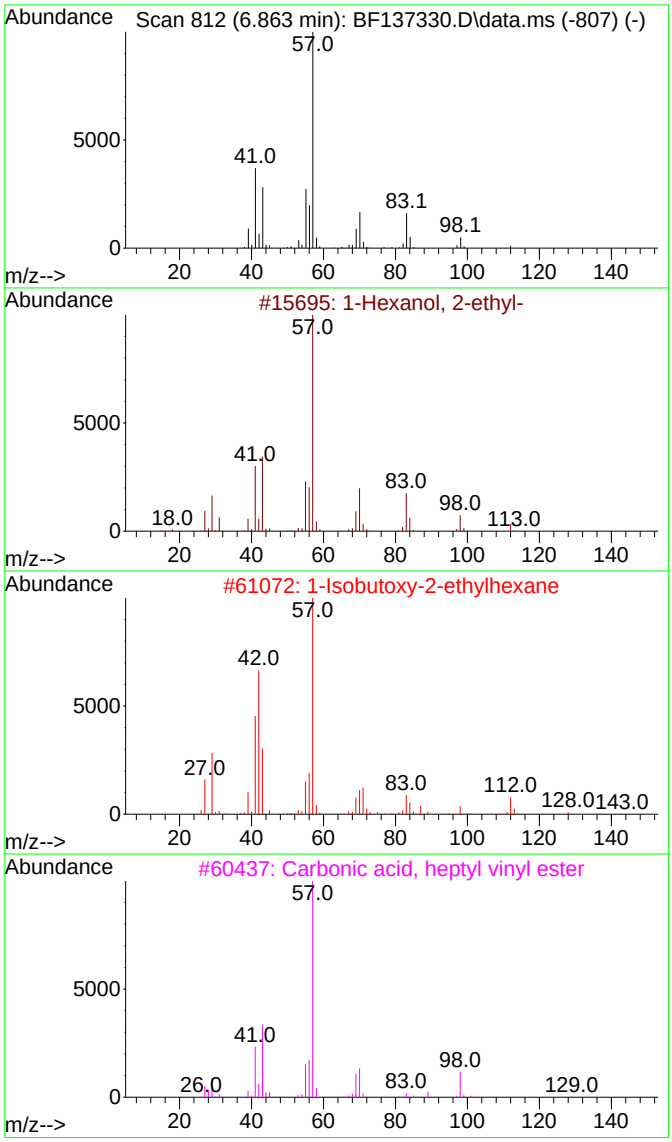
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

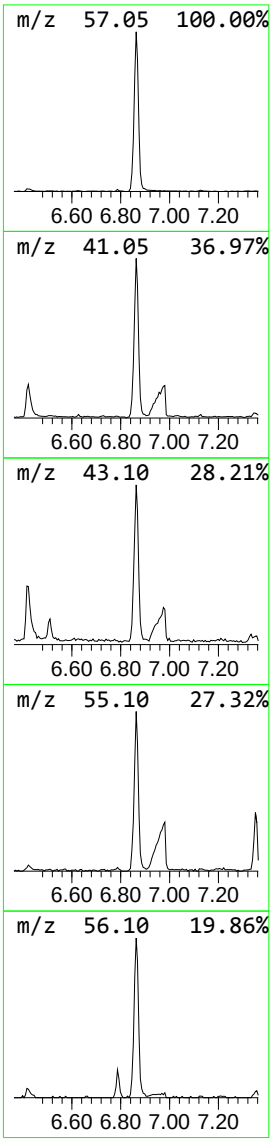
****

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.863	25.18 ng	406069	1,4-Dichlorobenzene-d4	6.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	74
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53
4	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	53
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020724\
Data File : BF137330.D
Acq On : 07 Feb 2024 20:04
Operator : CG\JU
Sample : P1342-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317AP-GW-20240131-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

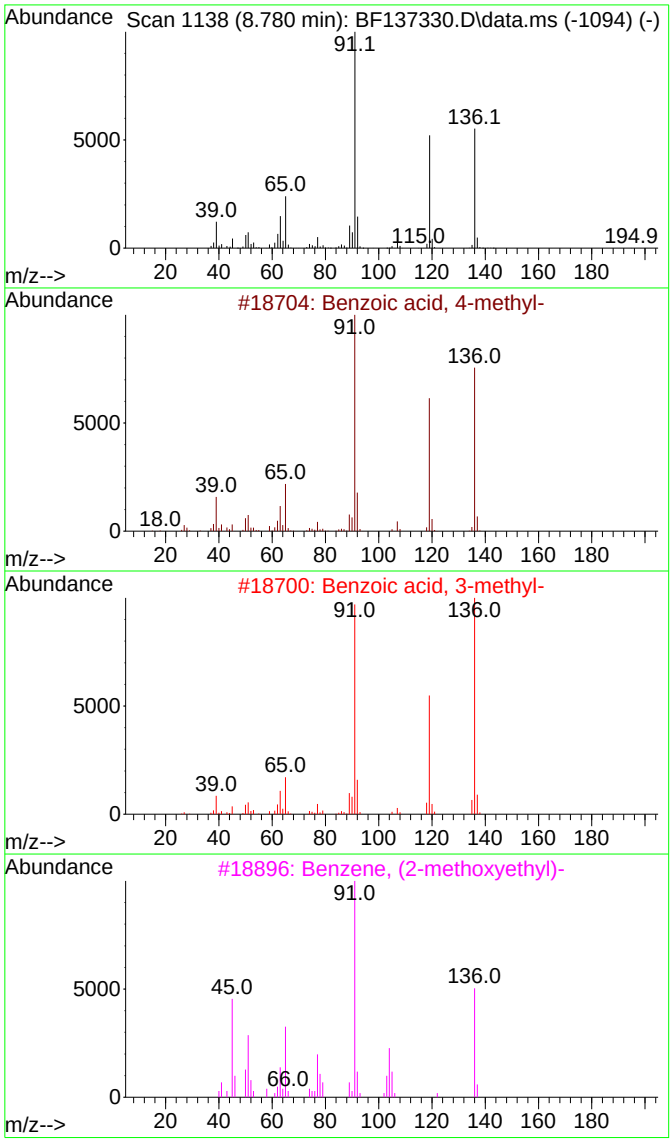
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

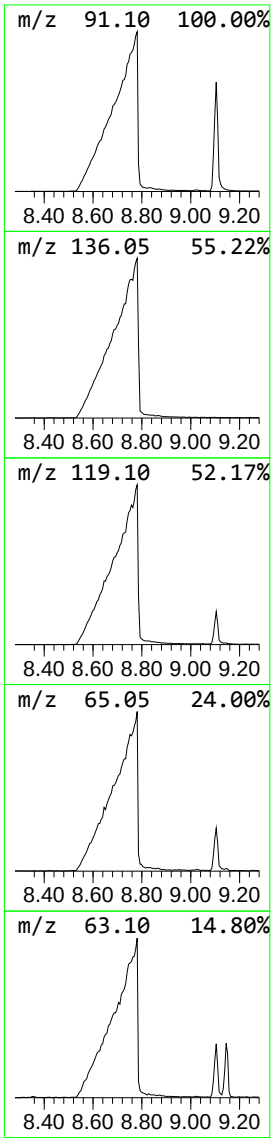
****

Peak Number 4 Benzoic acid, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.780	530.72 ng	15343500	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	97
2	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	91
3	Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	52
4	Ethanone, 2,2-dichloro-1-(4-meth...	202	C9H8Cl2O	004974-59-8	52
5	Benzoic acid, 4-methyl-, 1-methy...	192	C12H16O2	100556-51-2	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020724\
Data File : BF137330.D
Acq On : 07 Feb 2024 20:04
Operator : CG\JU
Sample : P1342-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317AP-GW-20240131-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

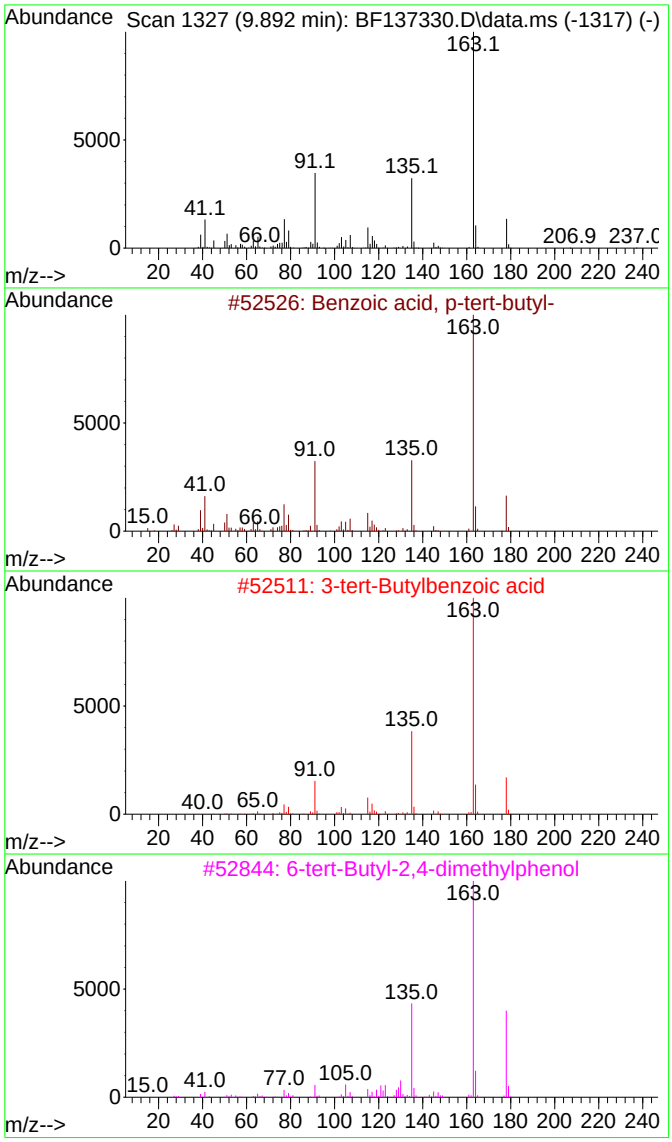
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

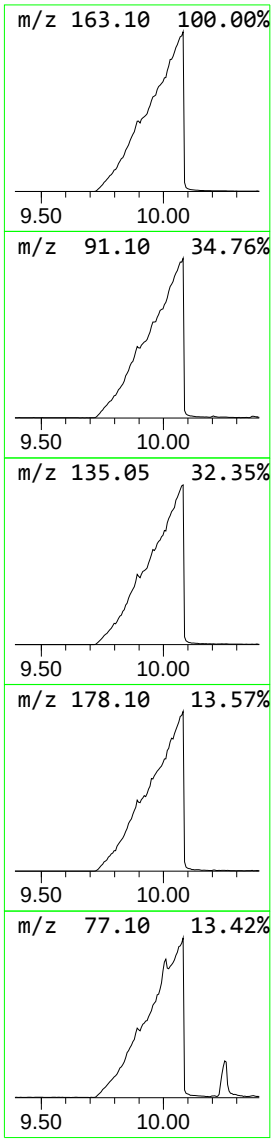
****

Peak Number 5 3-tert-Butylbenzoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.892	14.71 ng	3363170	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	95
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	94
3	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	68
4	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	59
5	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020724\
Data File : BF137330.D
Acq On : 07 Feb 2024 20:04
Operator : CG\JU
Sample : P1342-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317AP-GW-20240131-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

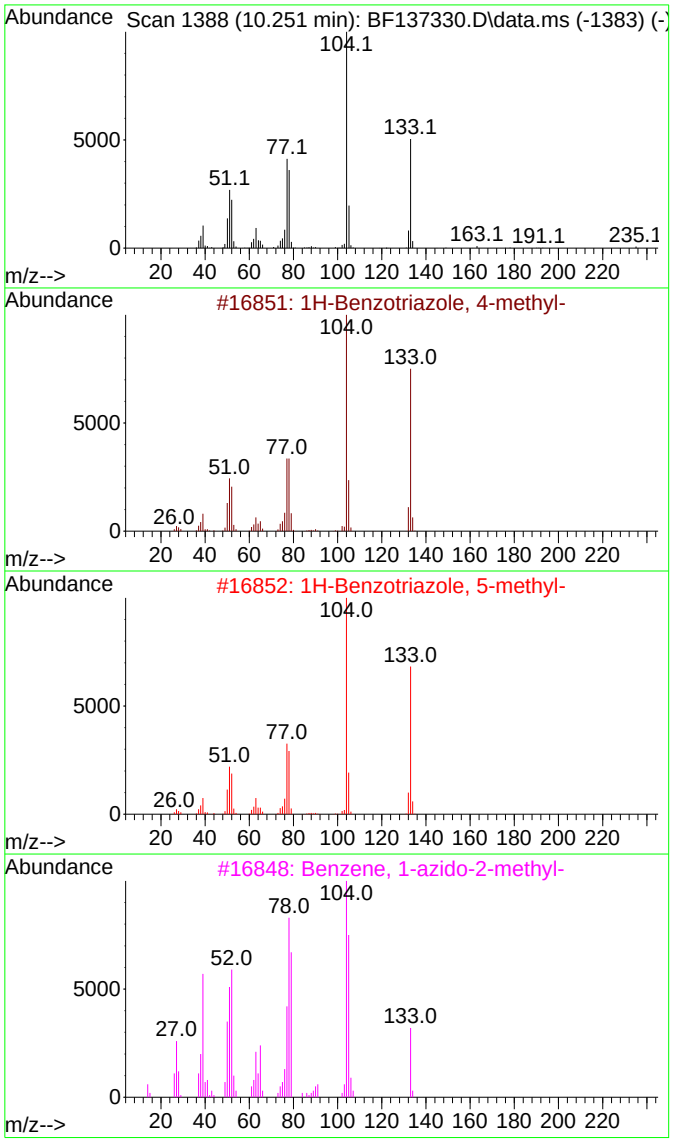
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

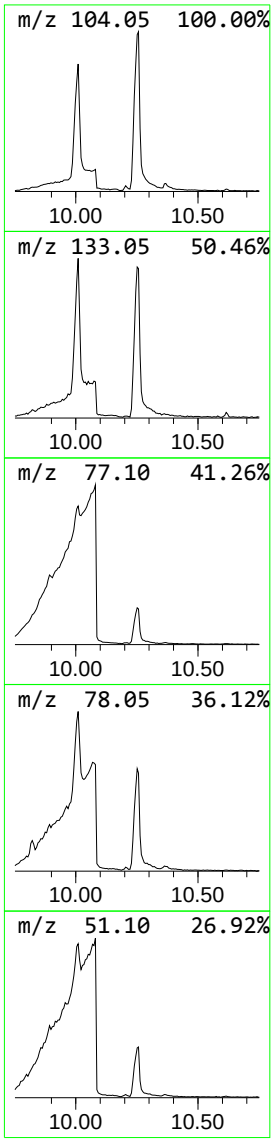
****

Peak Number 6 1H-Benzotriazole, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.251	4.00 ng	914998	Acenaphthene-d10	9.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	97
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	96
3	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	74
4	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	64
5	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020724\
Data File : BF137330.D
Acq On : 07 Feb 2024 20:04
Operator : CG\JU
Sample : P1342-09
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-317AP-GW-20240131-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-et...	6.863	25.2	ng	406069	1	6.786	322505	20.0
Benzoic acid, 4...	8.780	530.7	ng	15343500	2	8.069	578218	20.0
3-tert-Butylben...	9.892	14.7	ng	3363170	3	9.822	4571310	20.0
1H-Benzotriazol...	10.251	4.0	ng	914998	3	9.822	4571310	20.0