LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052823.D
Acq On : 25 Mar 2022 00:12
Operator : CG/JU
Sample : N2090-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-59

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_G\Methods\8270-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052823.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.169	126	133	140	rBV3	19717	37222	1.19%	0.316%
2	5.702	386	394	402	rVB	249400	408273	13.05%	3.470%
3	7.288	657	664	671	rBV	173436	292375	9.35%	2.485%
4	8.140	802	809	816	rBV	112307	192923	6.17%	1.640%
5	9.303	1000	1007	1021	rVB	405331	756533	24.19%	6.430%
6	10.954	1279	1288	1295	rBV	152235	287682	9.20%	2.445%
7	12.275	1505	1513	1519	rBV2	24831	44921	1.44%	0.382%
8	13.392	1695	1703	1710	rBV	1076227	1780005	56.91%	15.129%
9	14.549	1896	1900	1908	rBV3	36010	64157	2.05%	0.545%
10	14.760	1930	1936	1943	rVB2	270920	447902	14.32%	3.807%
11	16.247	2182	2189	2197	rBV	1115789	1775518	56.77%	15.091%
12	16.476	2224	2228	2237	rVB8	15639	34300	1.10%	0.292%
13	17.504	2397	2403	2409	rBV	375337	603156	19.28%	5.126%
14	18.385	2548	2553	2561	rBV2	52370	89956	2.88%	0.765%
15	18.555	2579	2582	2590	rVB9	16943	39274	1.26%	0.334%
16	19.912	2810	2813	2819	rVB	40419	56684	1.81%	0.482%
17	20.112	2840	2847	2853	rVB	2322601	3127625	100.00%	26.583%
18	21.428	3066	3071	3079	rVB3	88918	148526	4.75%	1.262%
19	21.792	3127	3133	3141	rVB	391254	669537	21.41%	5.691%
20	22.327	3221	3224	3230	rVB3	36368	53118	1.70%	0.451%
21	23.431	3407	3412	3422	rVB6	62593	130740	4.18%	1.111%
22	25.105	3688	3697	3710	rVB2	232597	725045	23.18%	6.162%

Sum of corrected areas: 11765472

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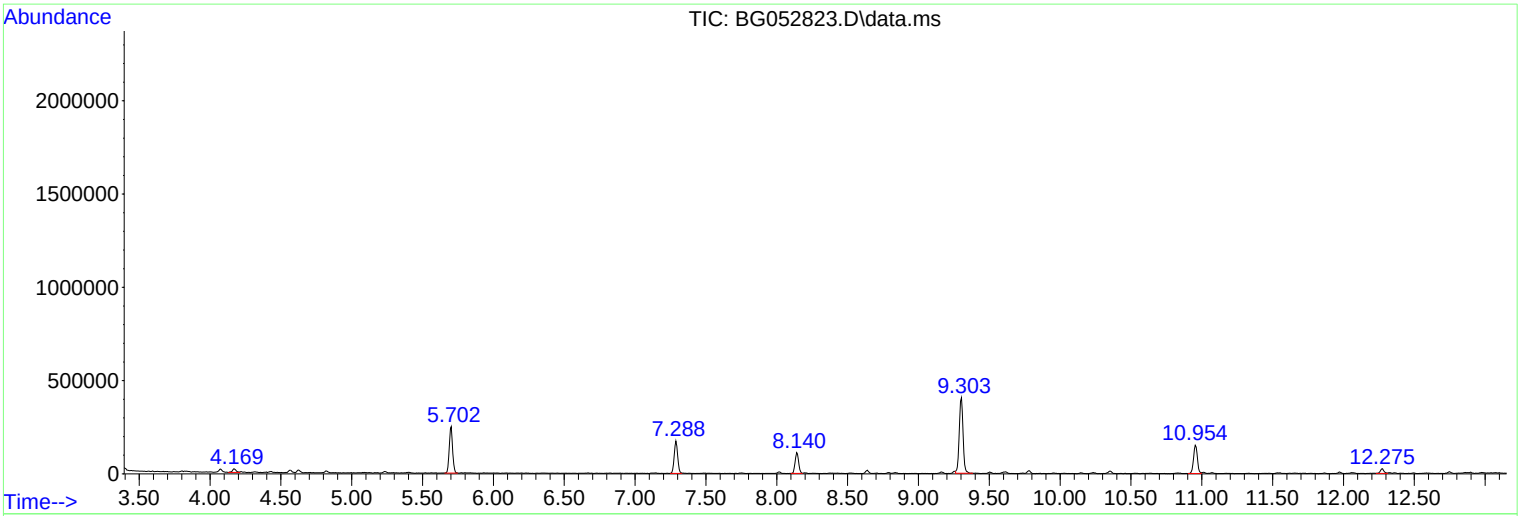
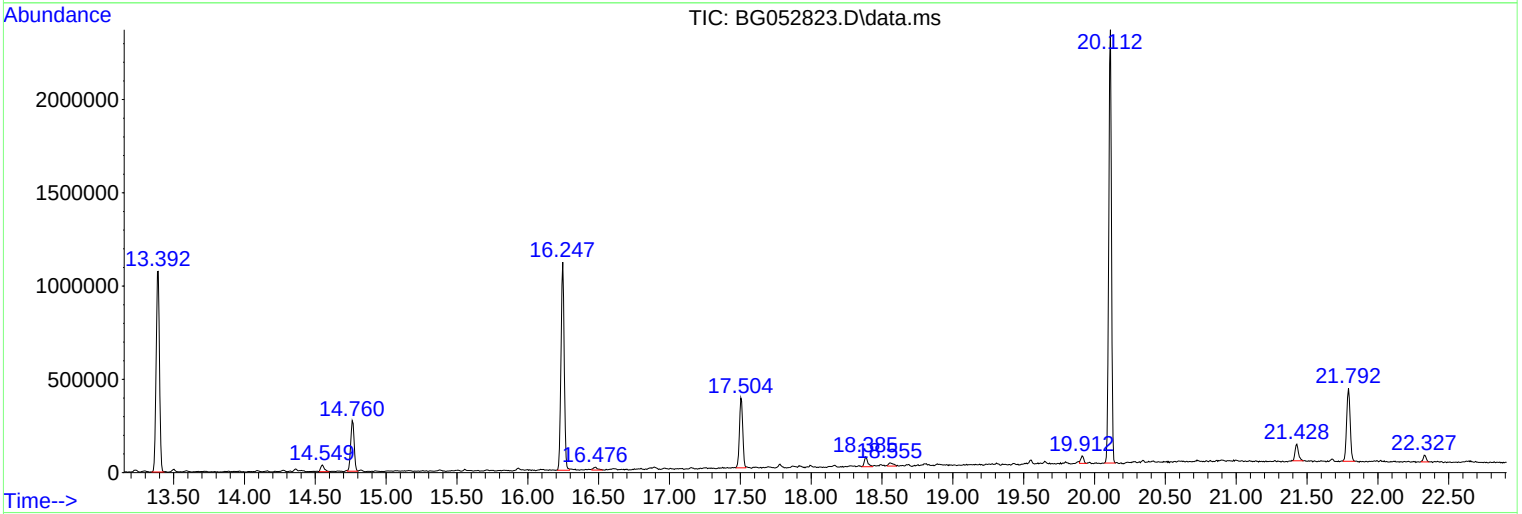
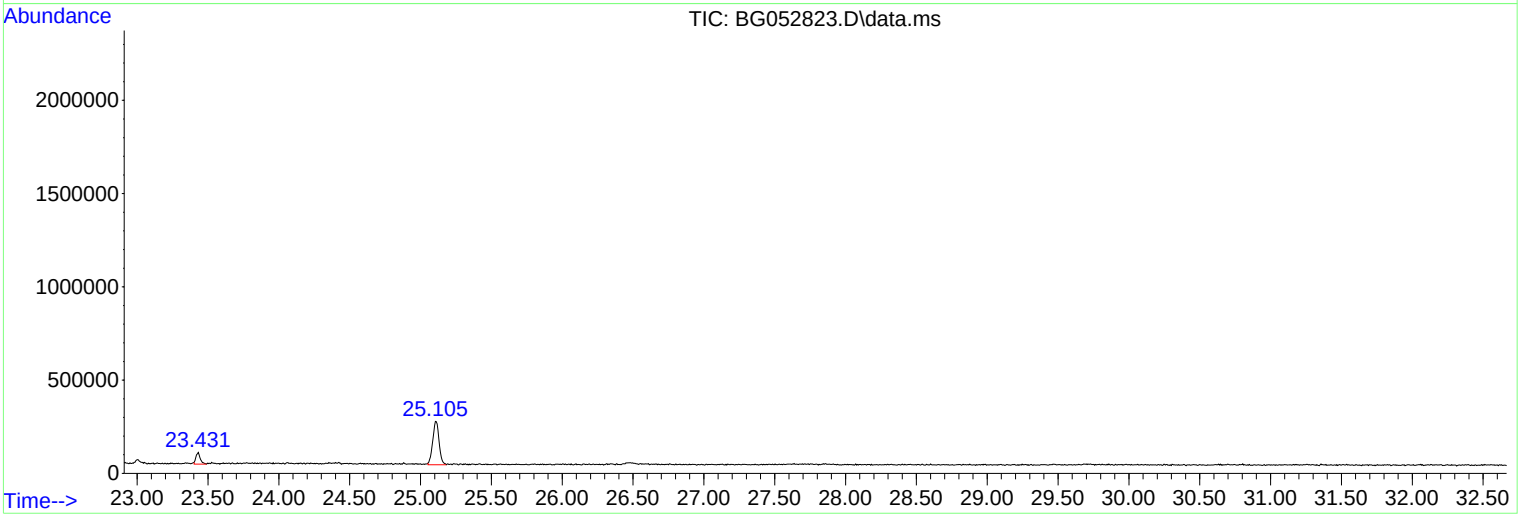
Instrument :
BNA_G
ClientSampleId :
MW-59

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

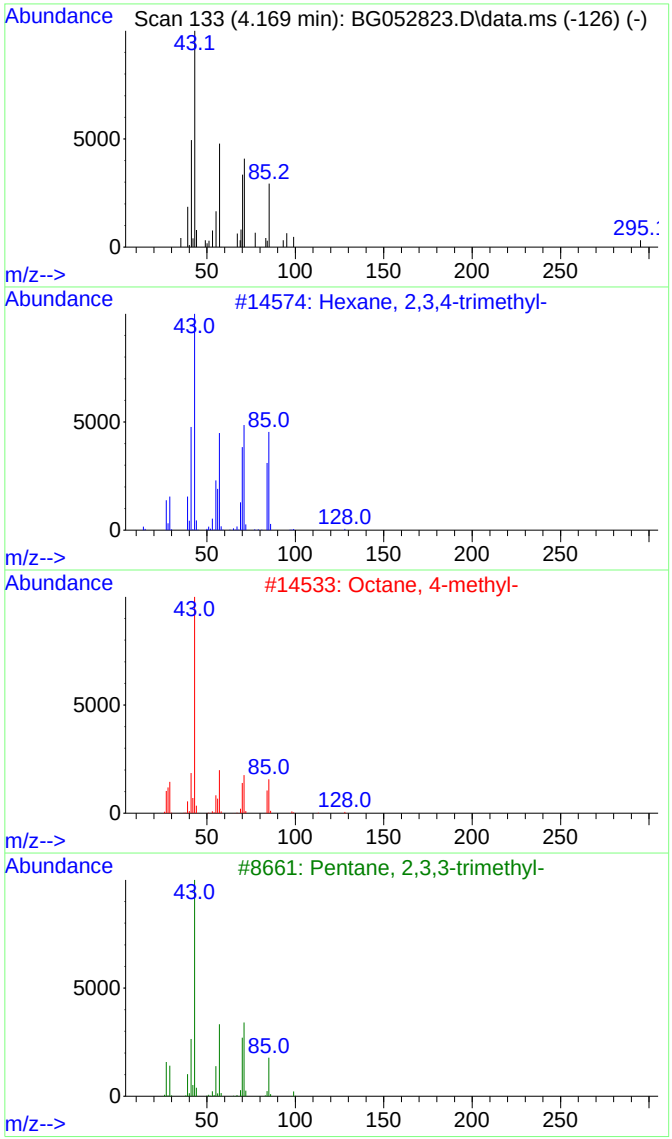
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

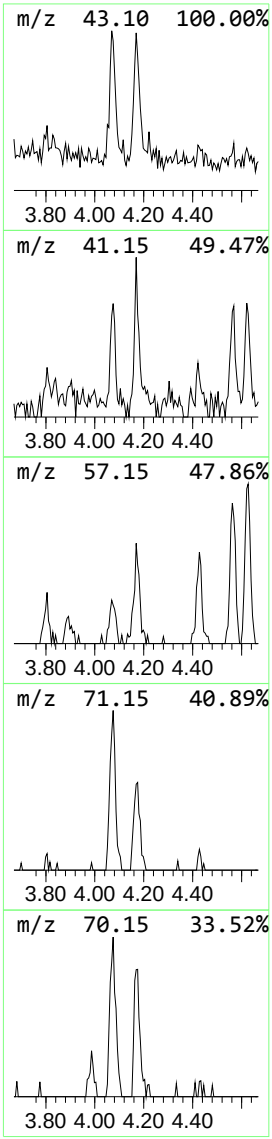
****

Peak Number 1 Hexane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.169	3.86 ng	37222	1,4-Dichlorobenzene-d4	8.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
2	Octane, 4-methyl-	128	C9H20	002216-34-4	64
3	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
4	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	50
5	Sulfurous acid, decyl 2-propyl e...	264	C13H28O3S	1000309-12-1	42





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Sample : N2090-15
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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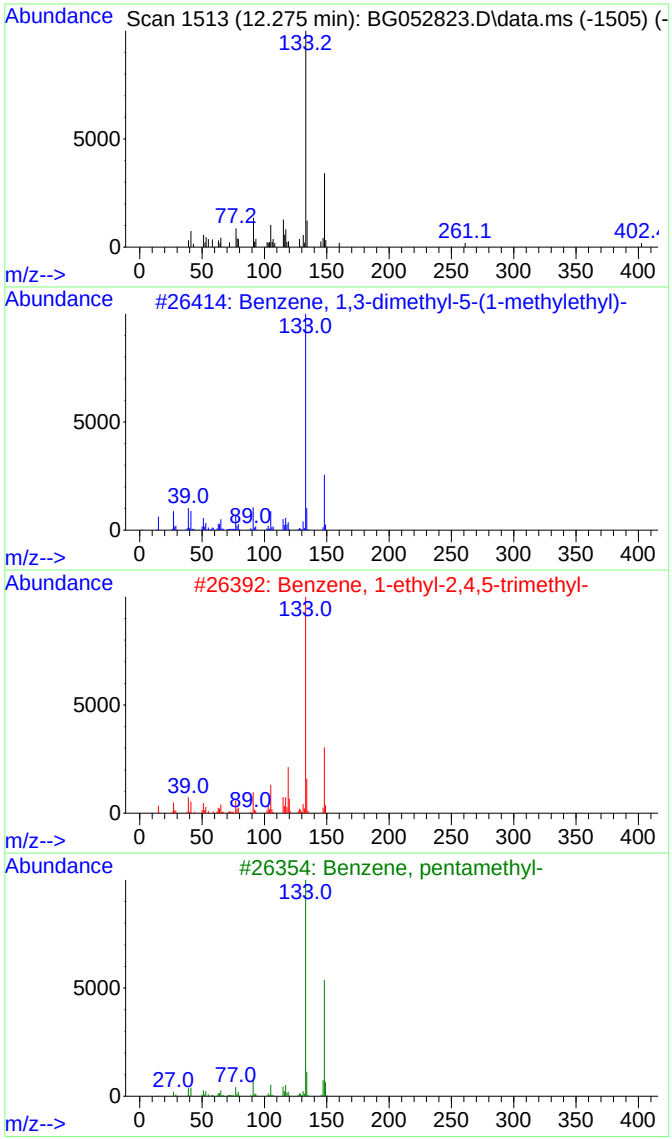
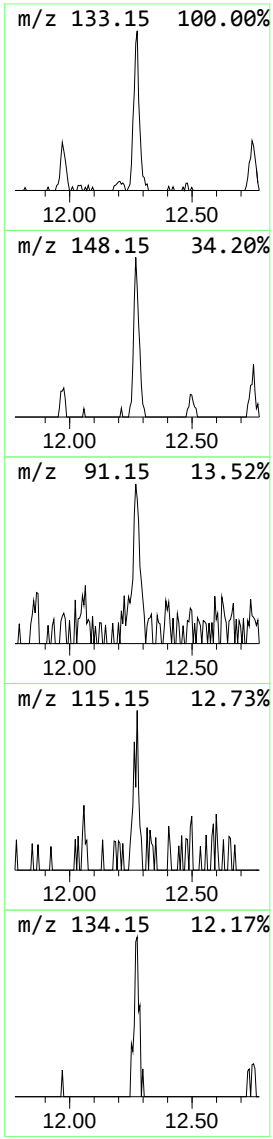
****
Peak Number 2 Benzene, 1,3-dimethyl-5-(1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.275	3.12 ng	44921	Naphthalene-d8	10.954

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	90
2	Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	017851-27-3	90
3	Benzene, pentamethyl-	148	C11H16	000700-12-9	87
4	3,4-Dimethylcumene	148	C11H16	1000370-34-1	87
5	1,5,6,7-Tetramethylbicyclo[3.2.0...	148	C11H16	134329-46-7	86





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Acq On : 25 Mar 2022 00:12
Operator : CG/JU
Sample : N2090-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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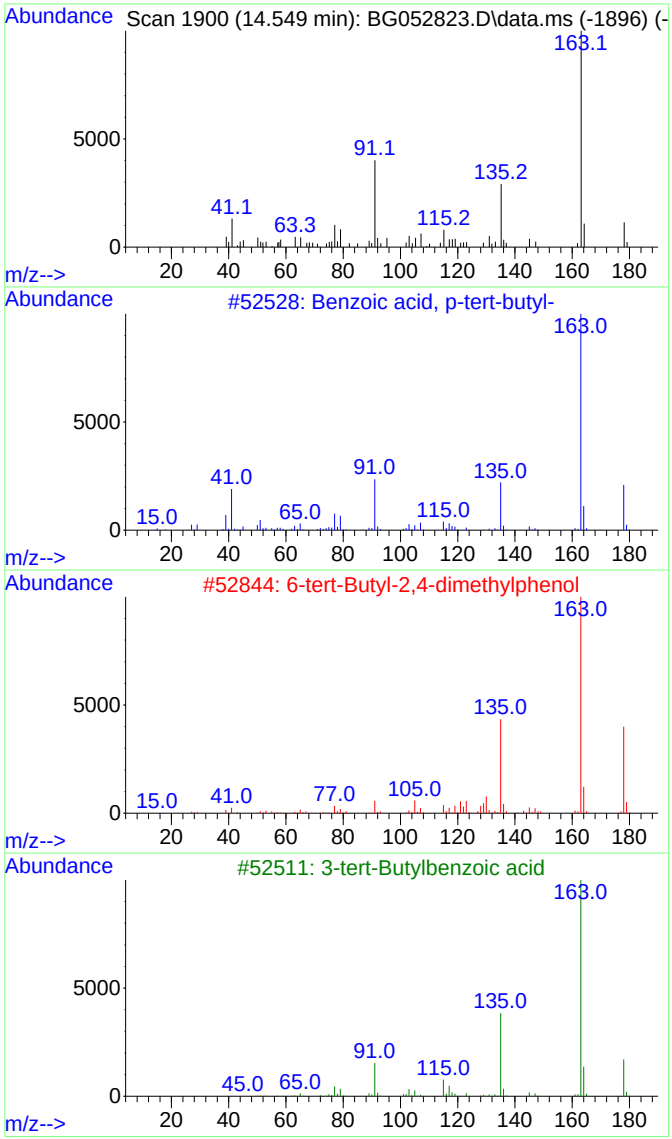
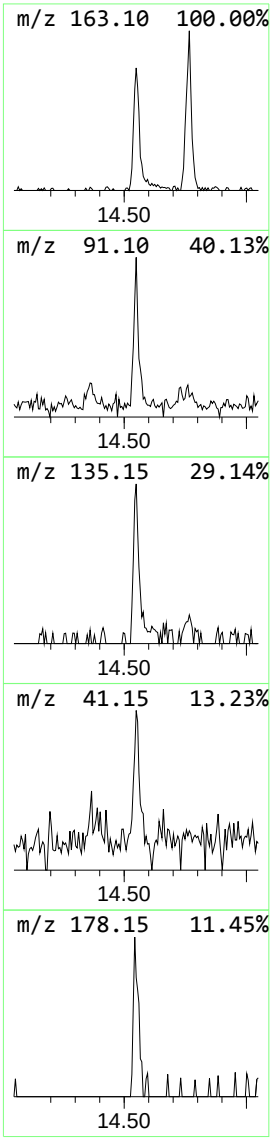
****

Peak Number 3 Benzoic acid, p-tert-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.549	2.86 ng	64157	Acenaphthene-d10	14.760

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	90
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	83
3	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	80
4	3-pyridinecarbonitrile, 2-amino-...	163	C8H9N3O	1010404-44-3	64
5	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	64





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Misc :
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Instrument :
BNA_G
ClientSampleId :
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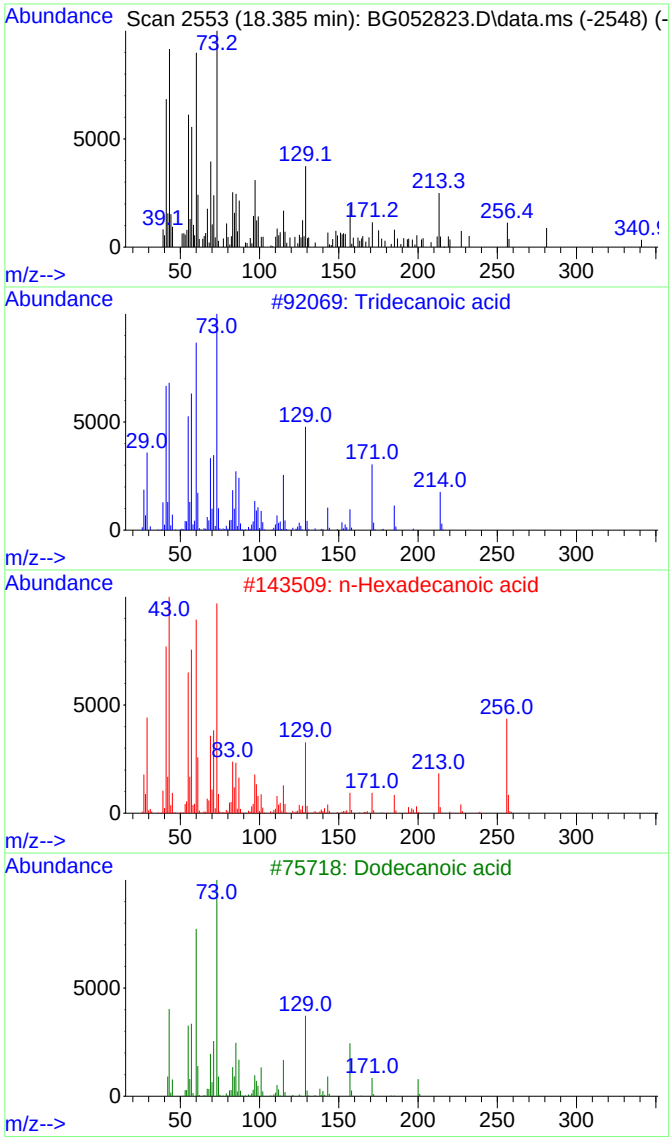
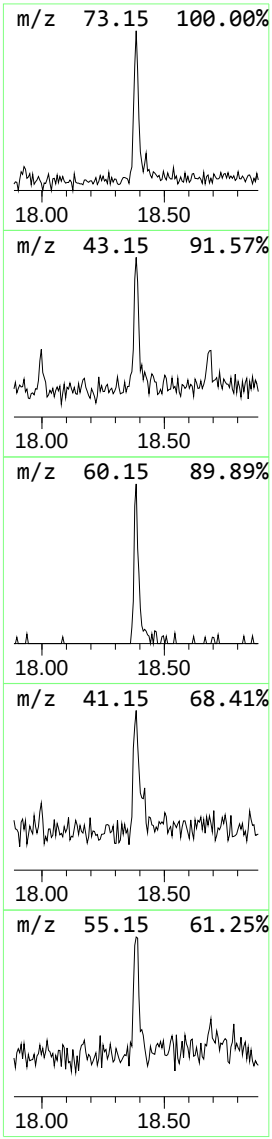
****

Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.385	2.98 ng	89956	Phenanthrene-d10	17.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47





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Misc :
ALS Vial : 18 Sample Multiplier: 1

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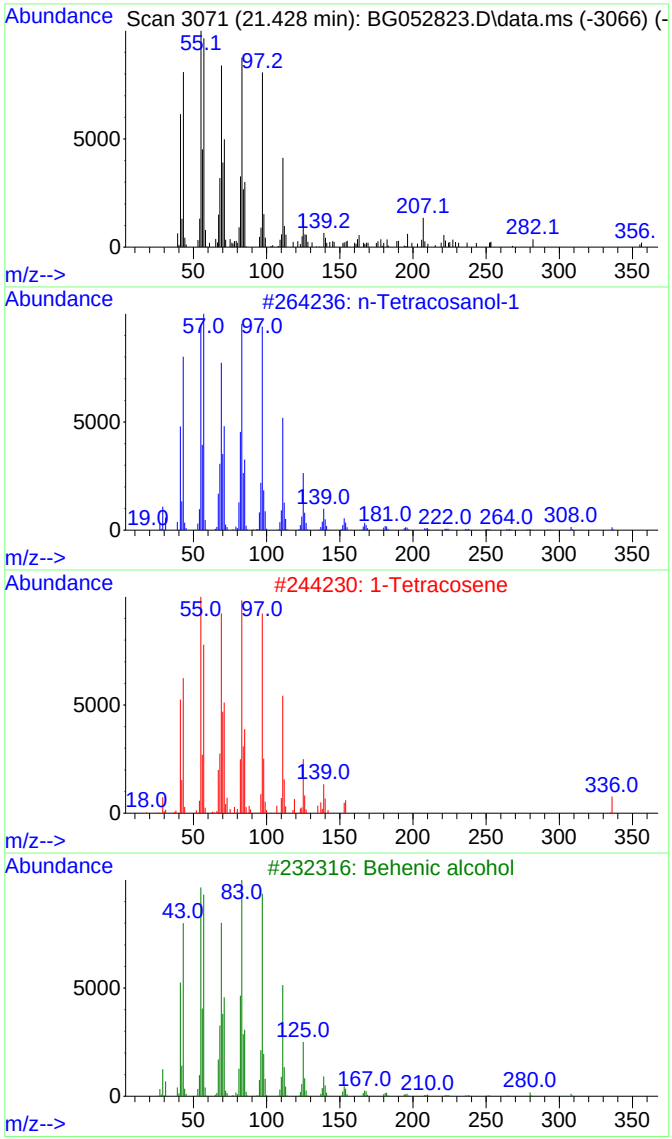
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

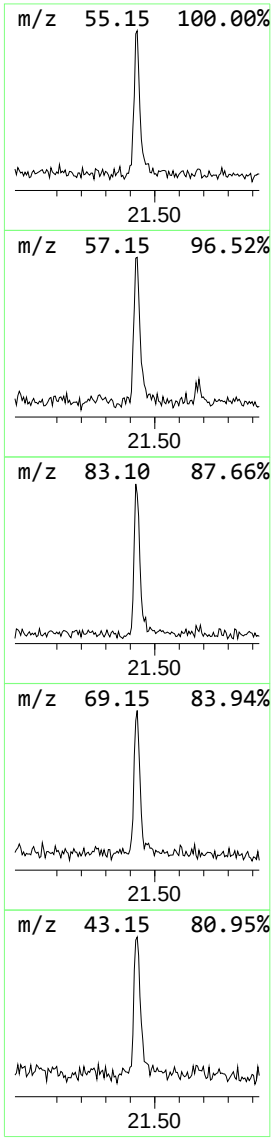
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.428	4.44 ng	148526	Chrysene-d12	21.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Tetracosene	336	C24H48	010192-32-2	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90





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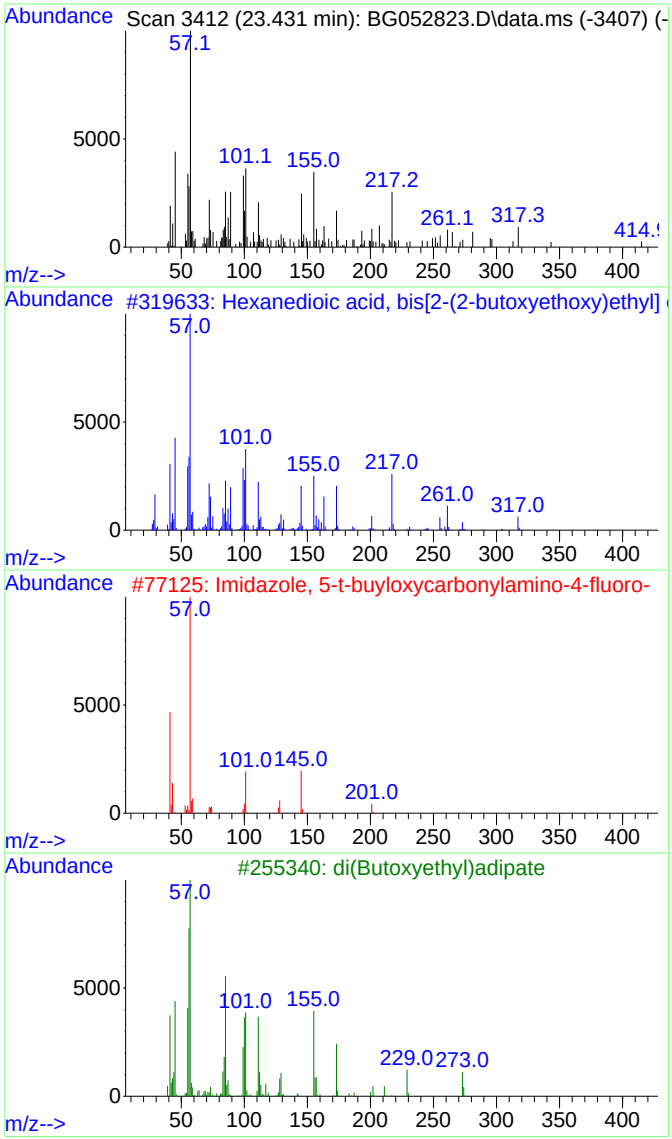
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

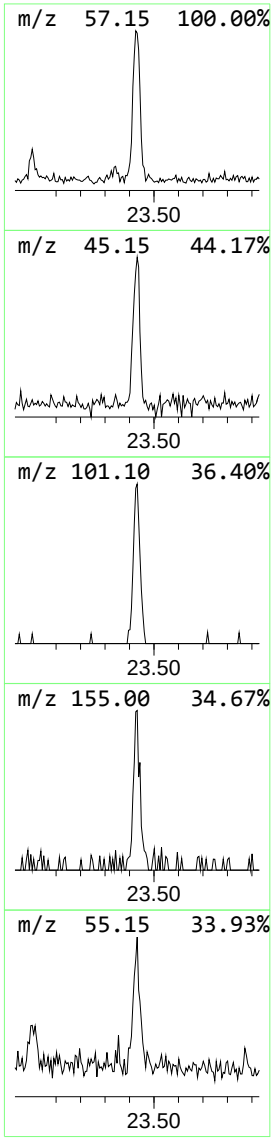
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexanedioic acid, bis[2-(2-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.431	3.91 ng	130740	Chrysene-d12	21.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	83
2	Imidazole, 5-t-buyloxycarbonylam...	201	C8H12FN3O2	330953-79-2	11
3	di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	9
4	3,4-Difluorothiophenol, S-trimet...	230	C11H12F2OS	1000470-51-6	9
5	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	9





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexane, 2,3,4-t...	4.169	3.9	ng	37222	1	8.140	192923	20.0
Benzene, 1,3-di...	12.275	3.1	ng	44921	2	10.954	287682	20.0
Benzoic acid, p...	14.549	2.9	ng	64157	3	14.760	447902	20.0
Tridecanoic acid	18.385	3.0	ng	89956	4	17.504	603156	20.0
n-Tetracosanol-1	21.428	4.4	ng	148526	5	21.792	669537	20.0
Hexanedioic aci...	23.431	3.9	ng	130740	5	21.792	669537	20.0