LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102620\
Data File : BF122117.D
Acq On : 26 Oct 2020 15:59
Operator : JU/CG
Sample : PB132611BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB132611BL

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	484	488	500	rVB	45432	78063	1.73%	0.278%
2	5.346	550	554	579	rBV	3073144	3403798	75.31%	12.123%
3	6.369	724	728	747	rBV	2917990	3401189	75.25%	12.114%
4	6.710	783	786	797	rBV	798378	714192	15.80%	2.544%
5	7.287	879	884	887	rBV	2288919	2375584	52.56%	8.461%
6	7.998	1000	1005	1012	rBV	936351	944836	20.90%	3.365%
7	9.075	1181	1188	1191	rBV	3854576	4143615	91.68%	14.758%
8	9.745	1297	1302	1309	rVB	1273050	1094425	24.21%	3.898%
9	10.022	1342	1349	1358	rVB	45760	64393	1.42%	0.229%
10	10.539	1432	1437	1441	rBV	2561474	2671133	59.10%	9.514%
11	10.681	1457	1461	1471	rVB	134772	193721	4.29%	0.690%
12	10.892	1493	1497	1507	rVB	98640	171204	3.79%	0.610%
13	11.233	1550	1555	1562	rBV	1264374	1140753	25.24%	4.063%
14	11.757	1639	1644	1650	rBV5	32119	67339	1.49%	0.240%
15	11.910	1663	1670	1672	rBV	241871	298989	6.62%	1.065%
16	11.933	1672	1674	1690	rVB2	230884	449226	9.94%	1.600%
17	12.822	1819	1825	1828	rBV	4461006	4519833	100.00%	16.098%
18	13.874	2000	2004	2011	rVB	1082459	991047	21.93%	3.530%
19	14.327	2075	2081	2085	rBV3	37216	54893	1.21%	0.196%
20	14.627	2128	2132	2135	rVB	43868	47201	1.04%	0.168%
21	14.939	2182	2185	2190	rVB	73379	82755	1.83%	0.295%
22	15.304	2241	2247	2261	rVB	719278	994369	22.00%	3.542%
23	15.698	2310	2314	2321	rVB	60132	85003	1.88%	0.303%
24	16.163	2389	2393	2402	rVB	48733	89571	1.98%	0.319%

Sum of corrected areas: 28077132

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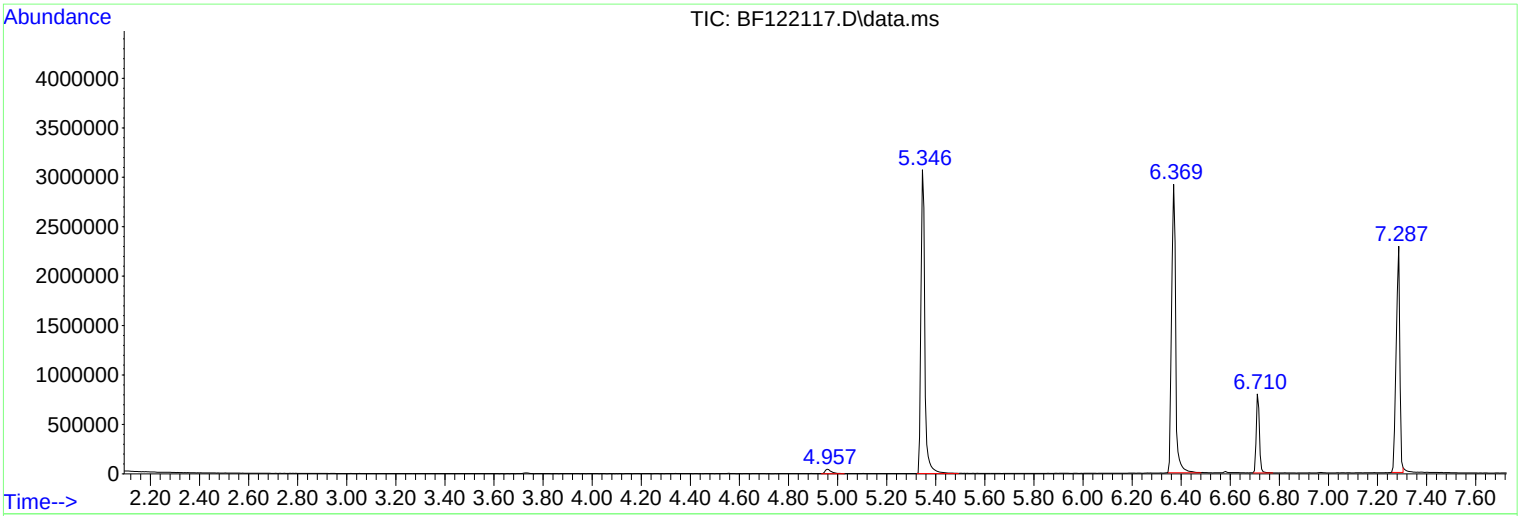
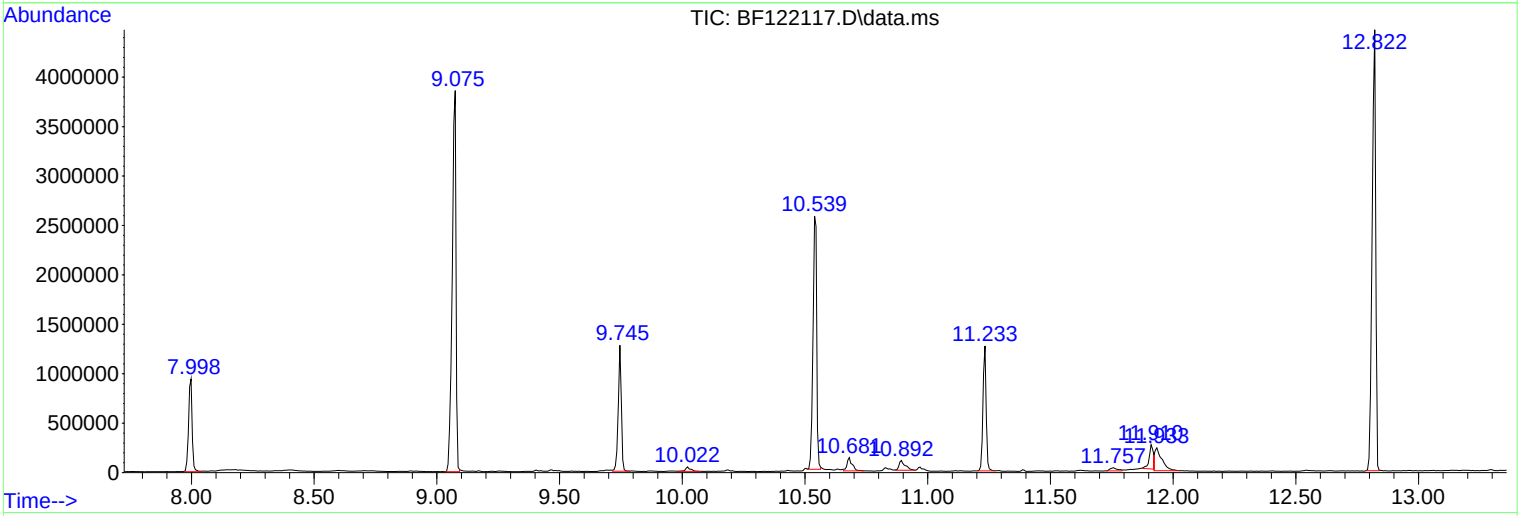
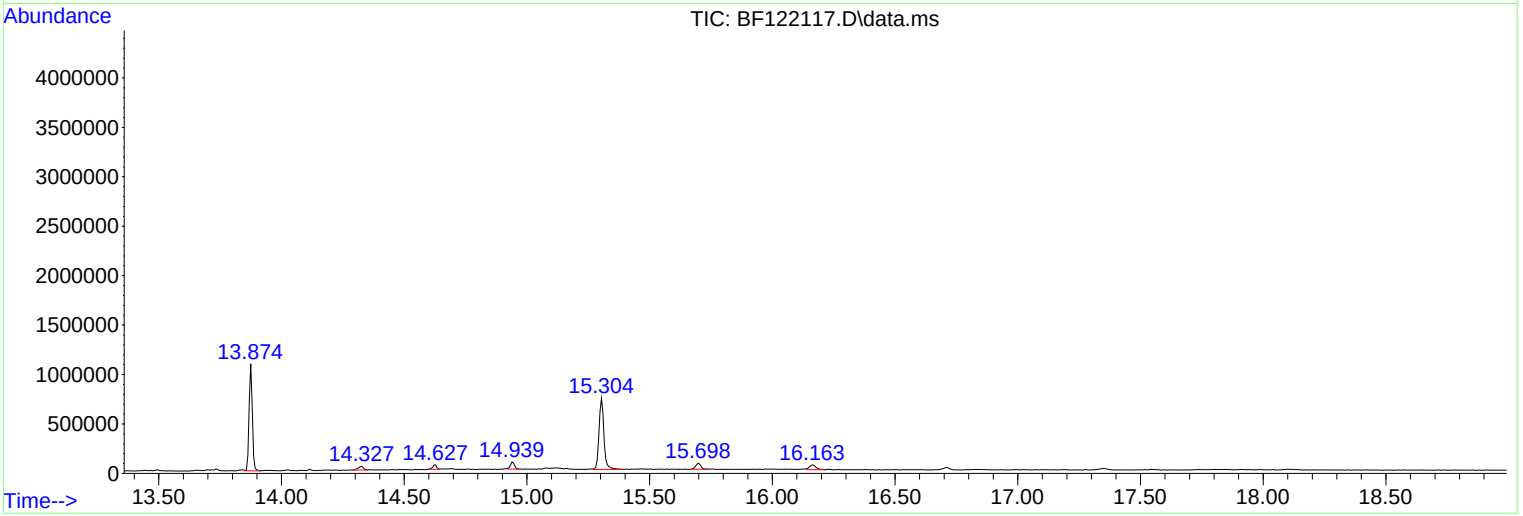
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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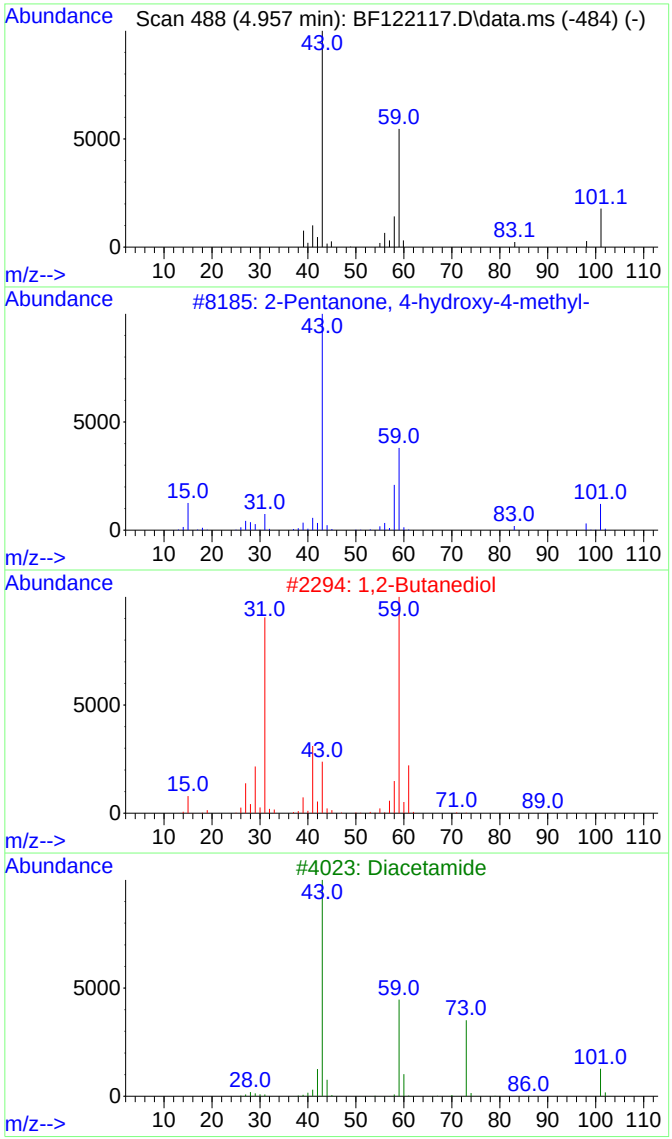
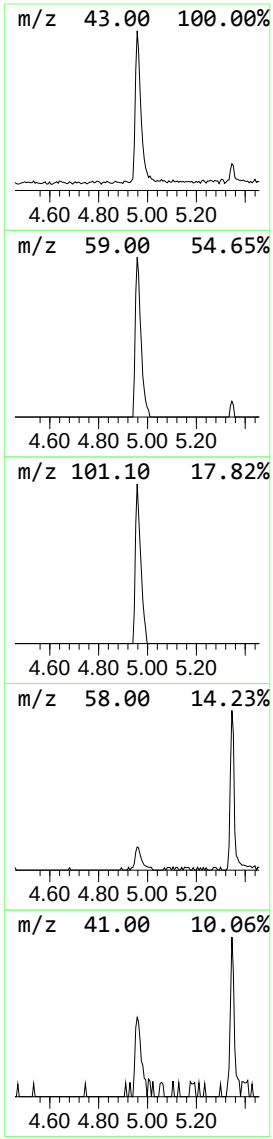
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	2.19 ng	78063	1,4-Dichlorobenzene-d4	6.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,2-Butanediol	90	C4H10O2	000584-03-2	38
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	3-Pentanol	88	C5H12O	000584-02-1	9





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ClientSampleId :
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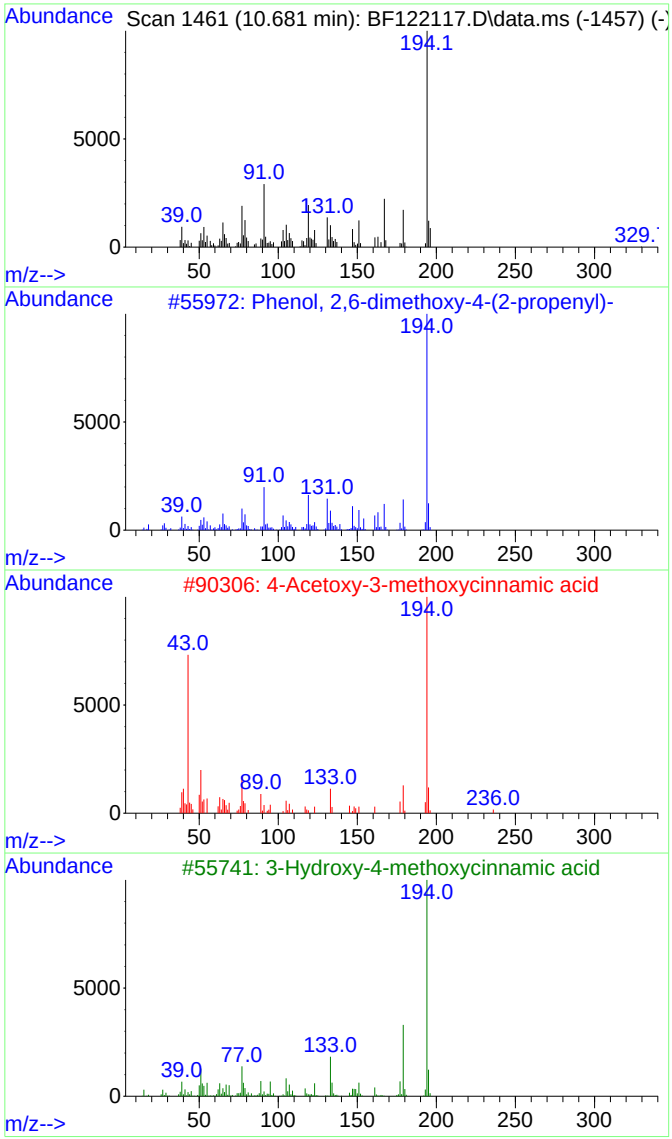
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

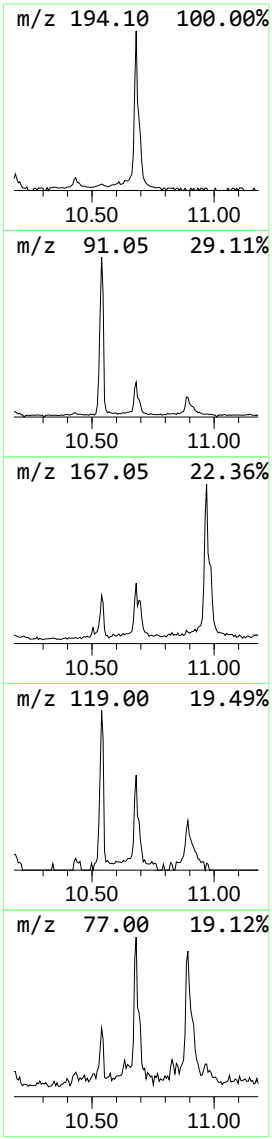
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Phenol, 2,6-dimethoxy-4-(2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.681	3.40 ng	193721	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dimethoxy-4-(2-prope...	194	C11H14O3	006627-88-9	81
2	4-Acetoxy-3-methoxycinnamic acid	236	C12H12O5	002596-47-6	50
3	3-Hydroxy-4-methoxycinnamic acid	194	C10H10O4	000537-73-5	49
4	1H-Benzimidazole, 2-phenyl-	194	C13H10N2	000716-79-0	47
5	2-Propenoic acid, 3-(4-hydroxy-3...	194	C10H10O4	001135-24-6	46





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Sample : PB132611BL
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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB132611BL

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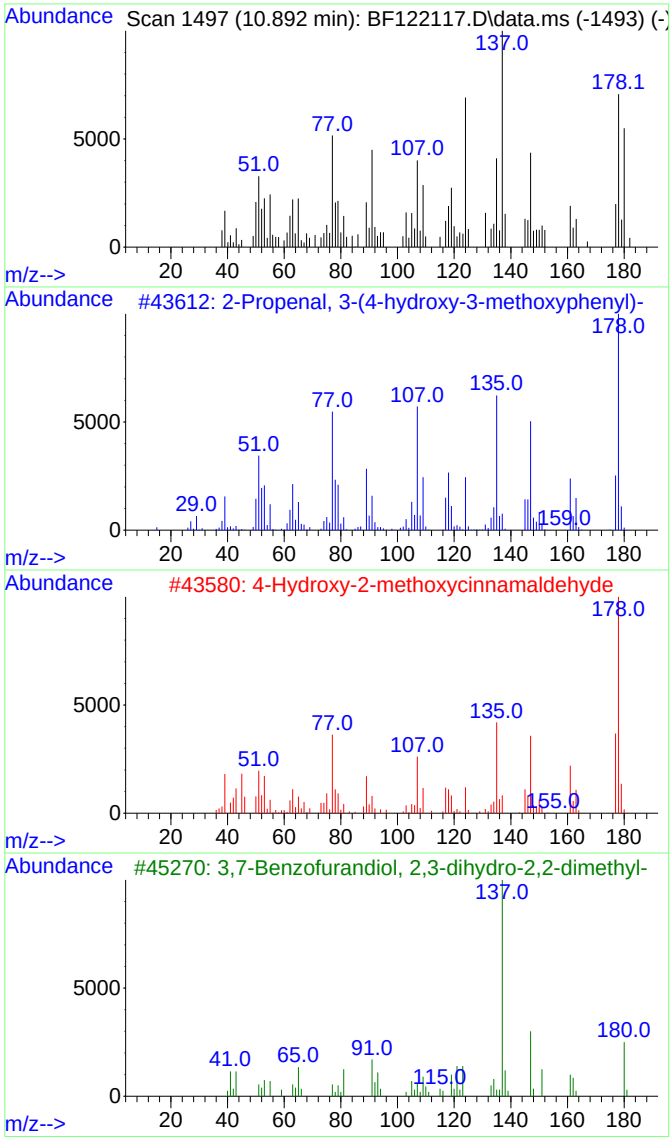
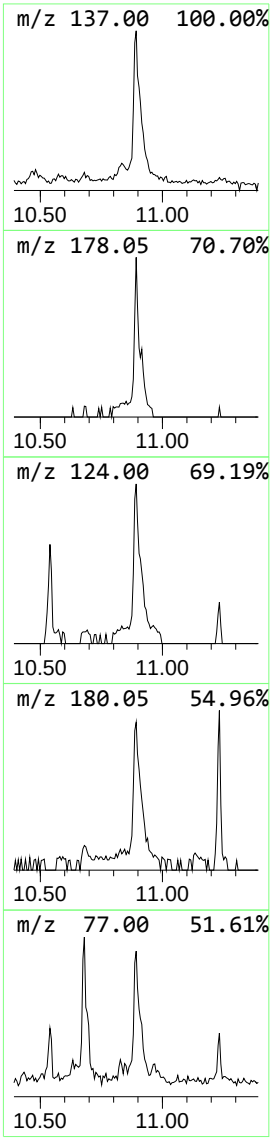
****
Peak Number 3 2-Propenal, 3-(4-hydroxy-3-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.892	3.00 ng	171204	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenal, 3-(4-hydroxy-3-metho...	178	C10H10O3	000458-36-6	96
2	4-Hydroxy-2-methoxycinnamaldehyde	178	C10H10O3	127321-19-1	87
3	3,7-Benzofurandiol, 2,3-dihydro-...	180	C10H12O3	017781-15-6	35
4	Benzene, 1-methyl-3-[(2-methylpr...	180	C11H16S	054576-36-2	18
5	Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	18





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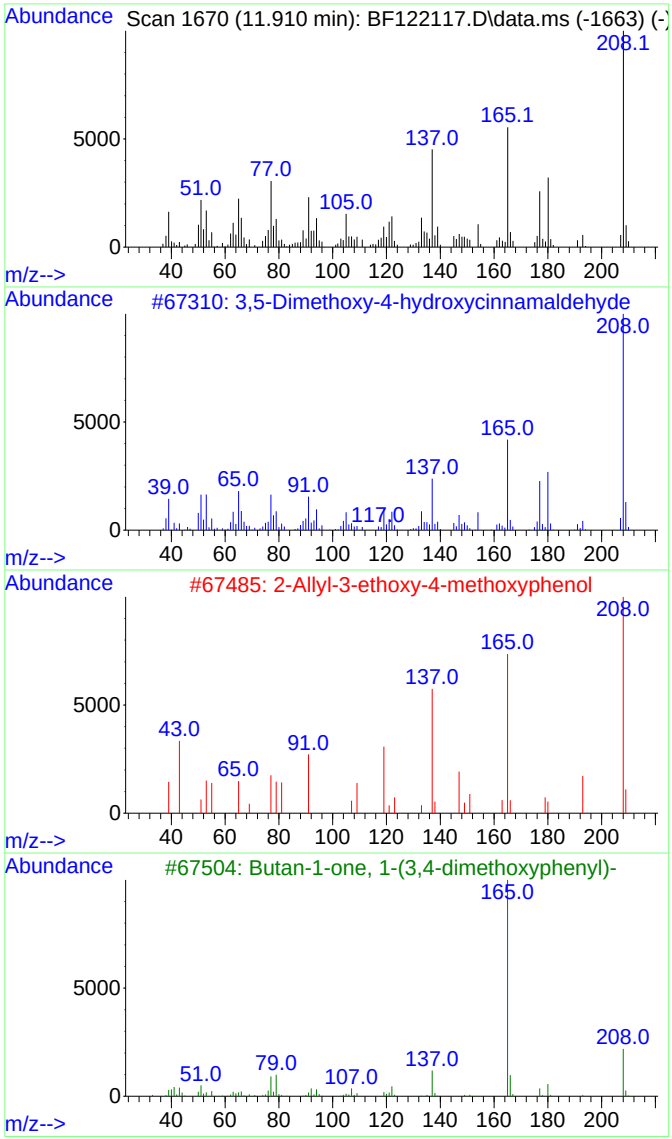
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

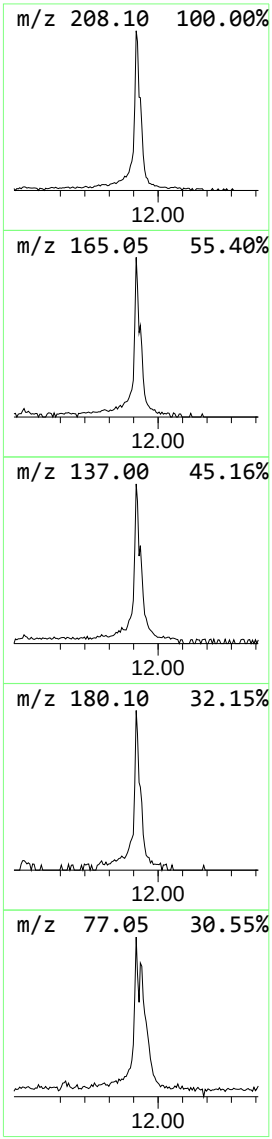
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	5.24 ng	298989	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	93
2	2-Allyl-3-ethoxy-4-methoxyphenol	208	C12H16O3	1000122-70-6	58
3	Butan-1-one, 1-(3,4-dimethoxyphe...	208	C12H16O3	054419-21-5	49
4	Imidazo[5,4-e][1,4]diazepine-4,7...	208	C9H12N4O2	144105-22-6	49
5	1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	45





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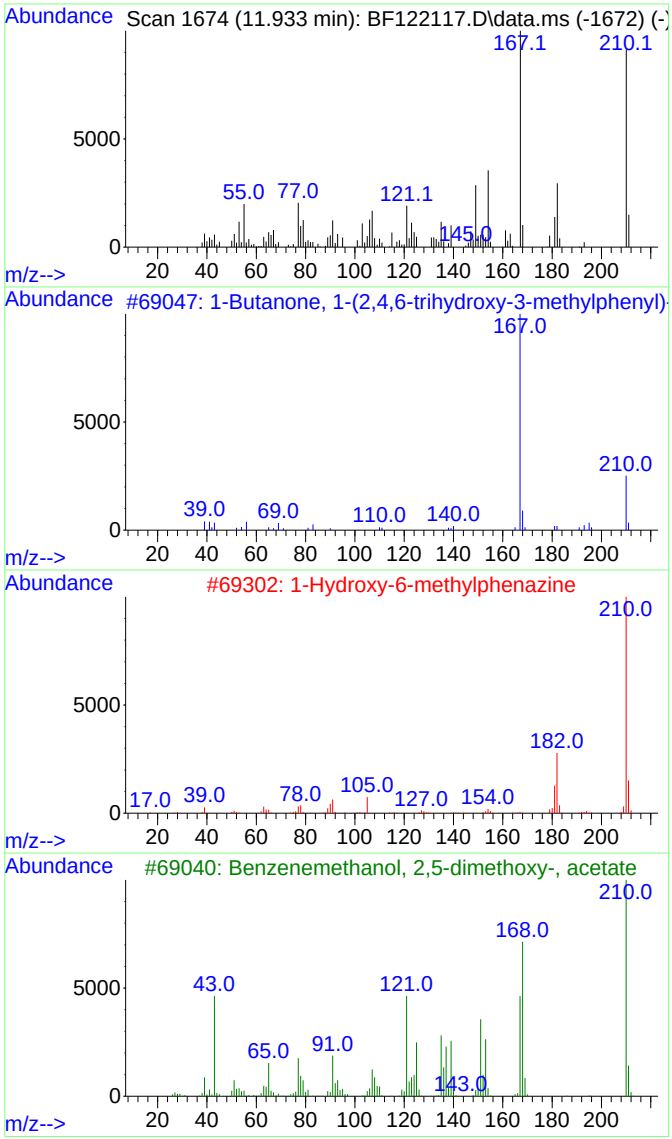
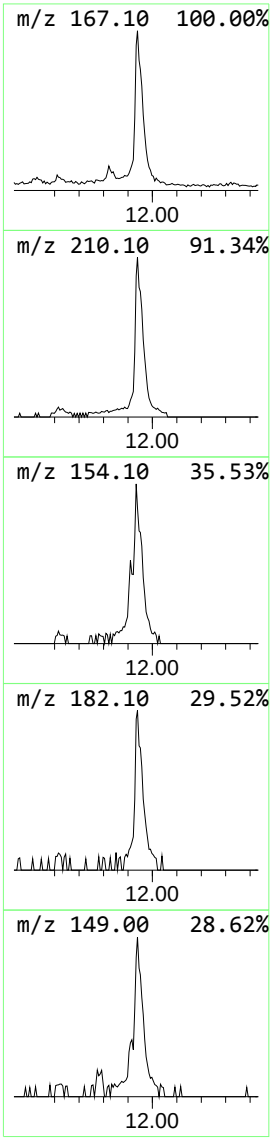
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Butanone, 1-(2,4,6-trihyd... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	7.88 ng	449226	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanone, 1-(2,4,6-trihydroxy-...	210	C11H14O4	001509-06-4	50
2	1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	46
3	Benzenemethanol, 2,5-dimethoxy-,...	210	C11H14O4	067698-75-3	41
4	1H-Naphtho[2,1-b]pyran-1-one, 3-...	210	C14H10O2	005891-82-7	38
5	Benzene, 1-methyl-4-(phenylmethyl)-	182	C14H14	000620-83-7	38





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	2.2	ng	78063	1	6.710	714192	20.0
Phenol, 2,6-dim...	10.681	3.4	ng	193721	4	11.233	1140750	20.0
2-Propenal, 3-(...	10.892	3.0	ng	171204	4	11.233	1140750	20.0
3,5-Dimethoxy-4...	11.910	5.2	ng	298989	4	11.233	1140750	20.0
1-Butanone, 1-(...	11.933	7.9	ng	449226	4	11.233	1140750	20.0