LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102622\
Data File : BG055298.D
Acq On : 26 Oct 2022 13:54
Operator : CG/JU
Sample : N5231-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20221020

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-BG102422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055298.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.315	340	345	354	rBV	35880	54299	1.89%	0.484%
2	5.797	420	427	439	rVB	343742	551952	19.24%	4.920%
3	7.418	695	703	713	rBV	205646	367108	12.79%	3.272%
4	8.270	842	848	856	rBV	125070	211130	7.36%	1.882%
5	9.445	1040	1048	1058	rBV	449721	803368	28.00%	7.161%
6	11.102	1322	1330	1337	rBV	174080	308071	10.74%	2.746%
7	13.511	1733	1740	1747	rBV	1203580	1823263	63.54%	16.252%
8	14.886	1966	1974	1980	rBV	276819	429166	14.96%	3.825%
9	16.361	2218	2225	2233	rBV	1007686	1644156	57.30%	14.655%
10	17.618	2433	2439	2447	rVB	360265	548881	19.13%	4.892%
11	18.464	2579	2583	2589	rBV	44757	82528	2.88%	0.736%
12	19.533	2760	2765	2775	rVB3	14653	37444	1.30%	0.334%
13	20.192	2871	2877	2885	rBV	2189479	2869297	100.00%	25.575%
14	20.503	2926	2930	2936	rVB	18786	32687	1.14%	0.291%
15	21.490	3095	3098	3108	rVB2	41117	93716	3.27%	0.835%
16	21.584	3110	3114	3119	rVB	58579	82258	2.87%	0.733%
17	21.895	3160	3167	3173	rBV2	362306	625716	21.81%	5.577%
18	25.291	3736	3745	3756	rVB2	220371	653956	22.79%	5.829%

Sum of corrected areas: 11218996

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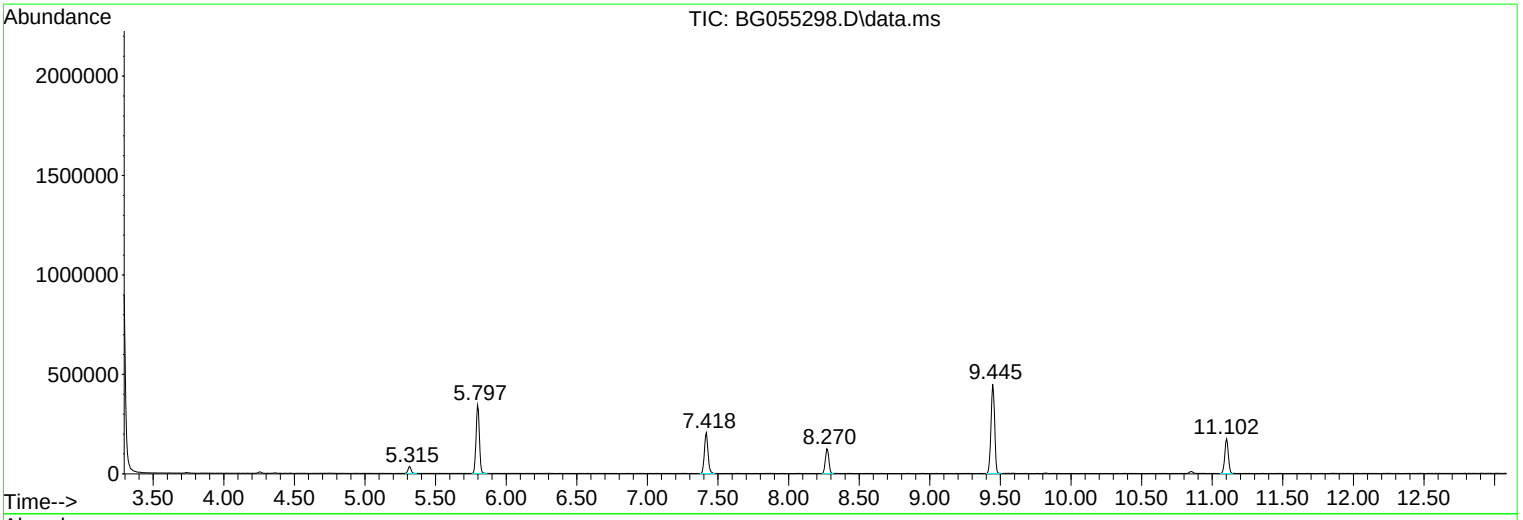
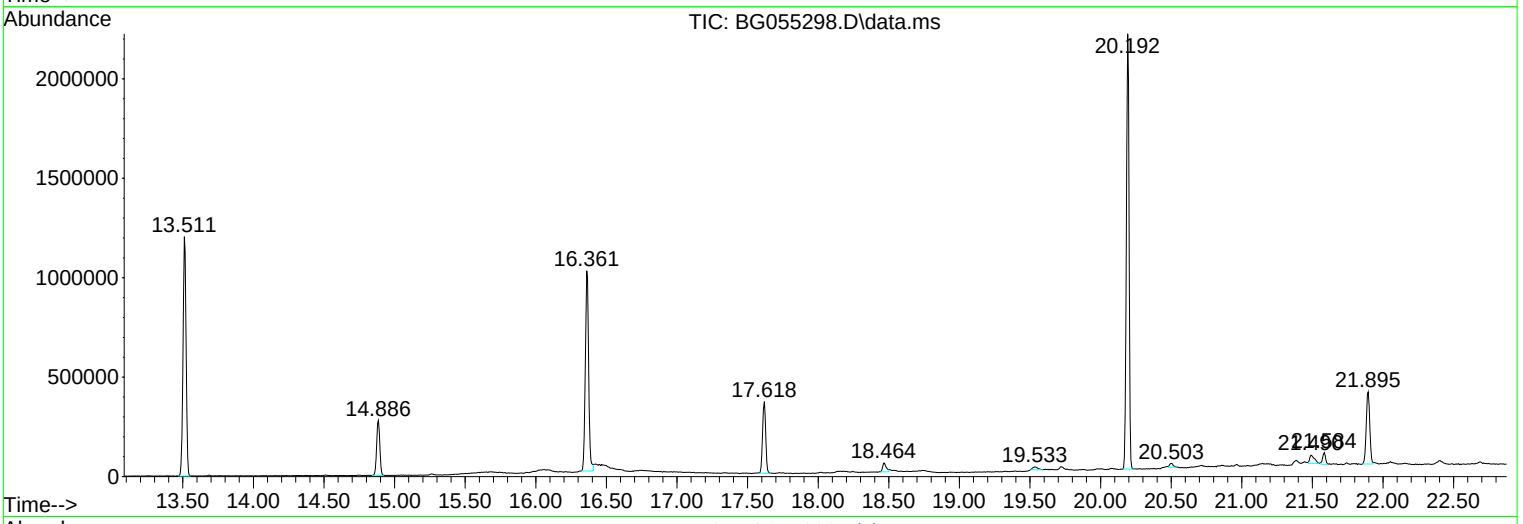
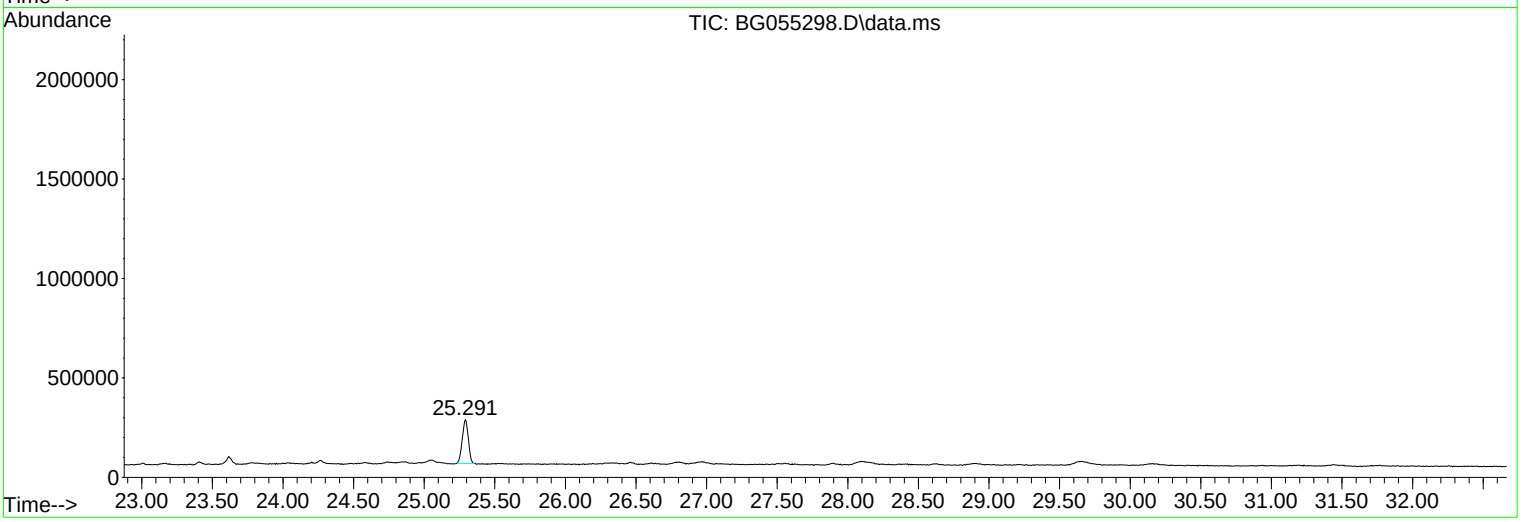
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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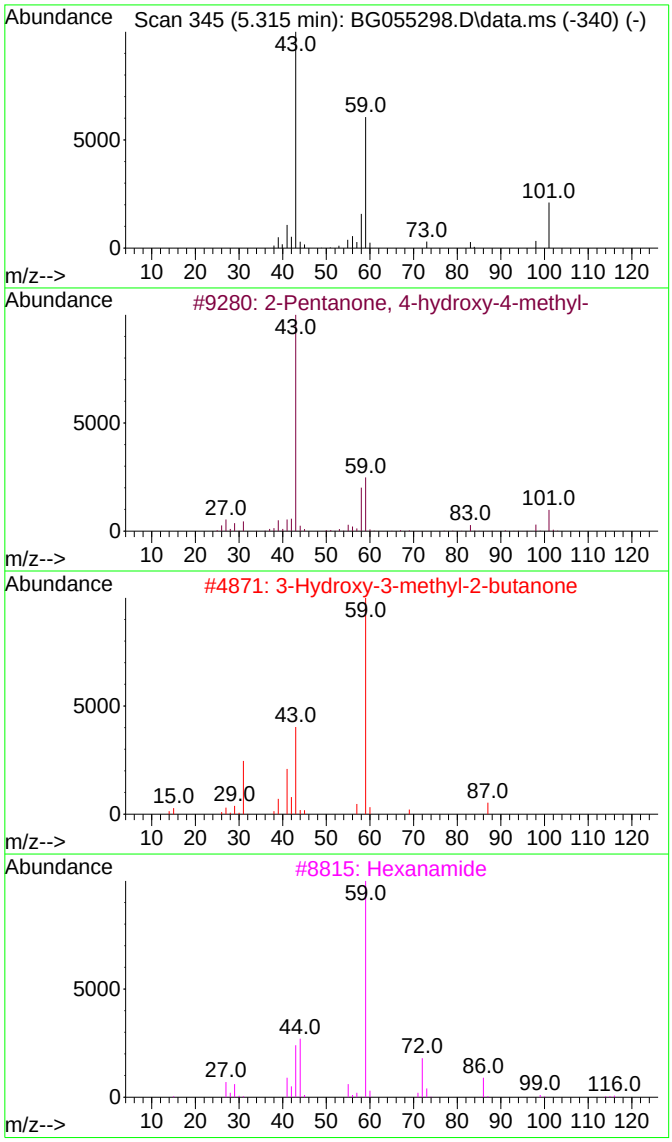
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

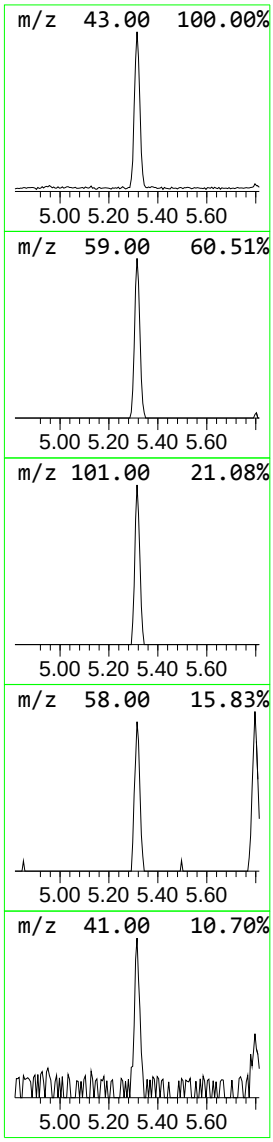
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.315	5.14 ng	54299	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3	Hexanamide	115	C6H13NO	000628-02-4	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

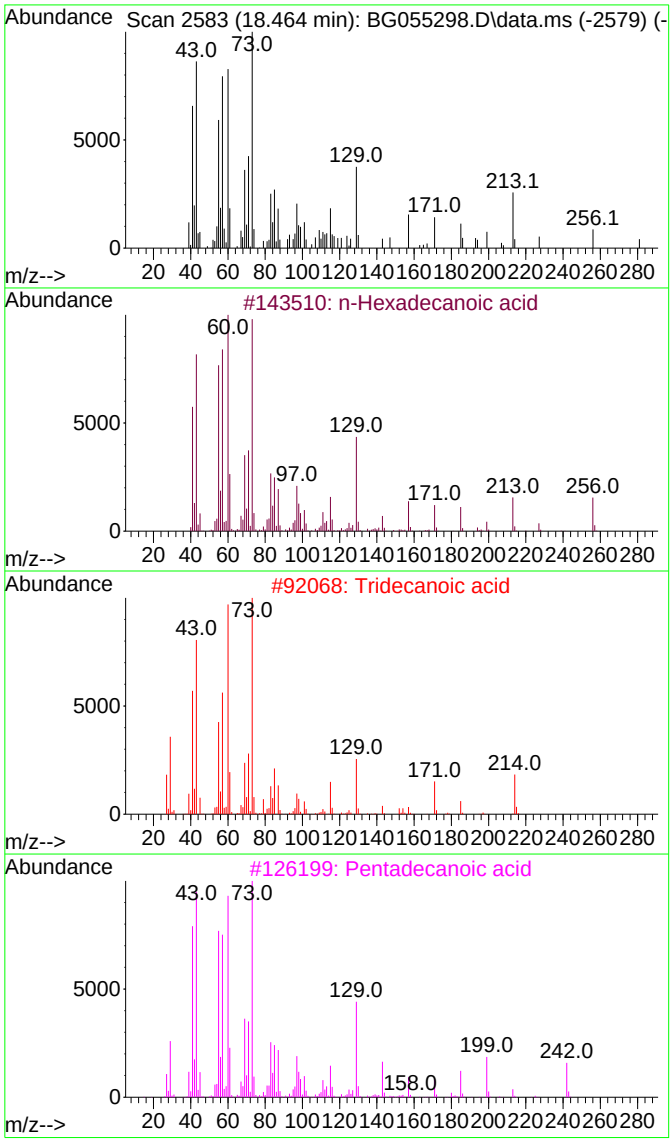
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

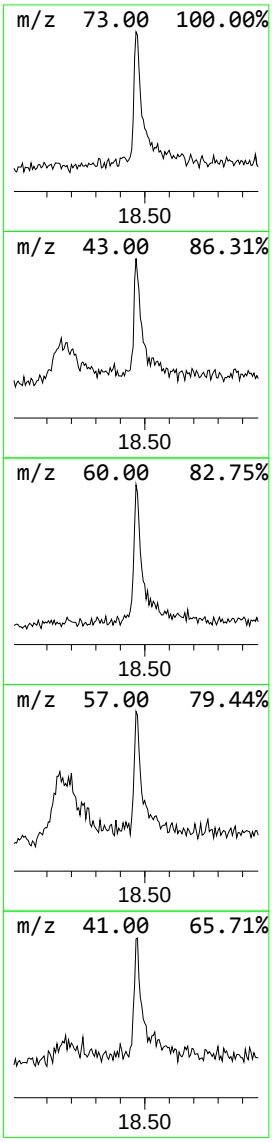
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.464	3.01 ng	82528	Phenanthrene-d10	17.618

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





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Sample : N5231-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-303-20221020

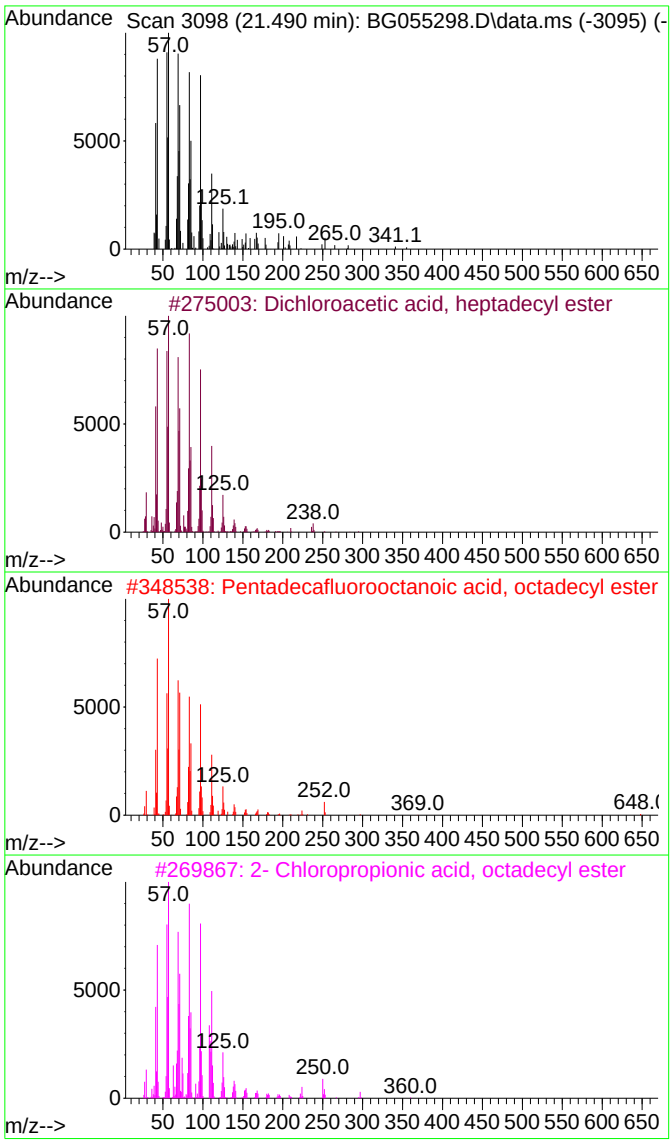
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG102422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

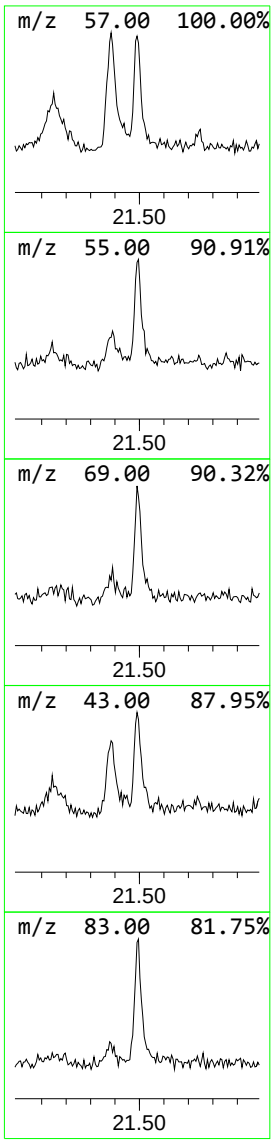
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.490	3.00 ng	93716	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91





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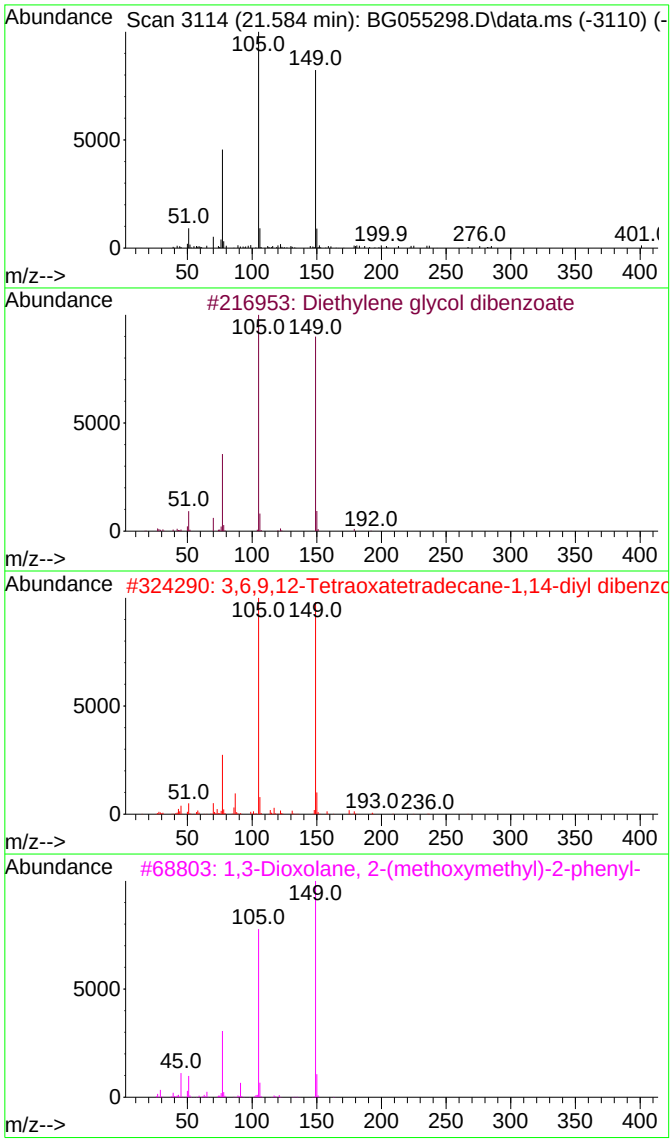
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

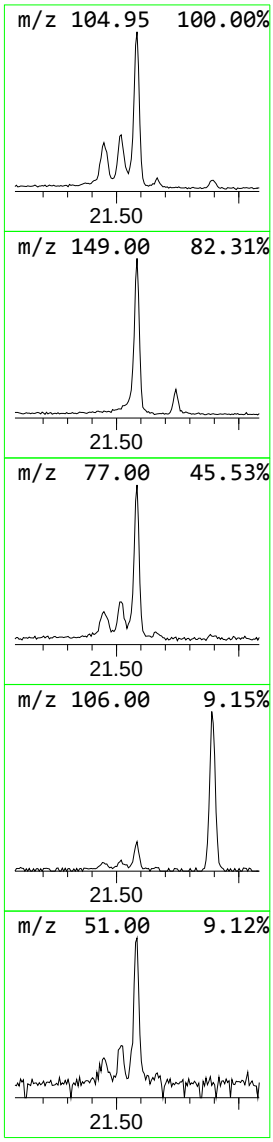
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.584	2.63 ng	82258	Chrysene-d12	21.895

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	64
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
4	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	47
5	2,5-Pyrrolidinedione, 1-(benzoyl...	219	C11H9NO4	023405-15-4	35





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.315	5.1	ng	54299	1	8.270	211130	20.0
n-Hexadecanoic ...	18.464	3.0	ng	82528	4	17.618	548881	20.0
Dichloroacetic ...	21.490	3.0	ng	93716	5	21.895	625716	20.0
Diethylene glyc...	21.584	2.6	ng	82258	5	21.895	625716	20.0