LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081823\
Data File : BF134851.D
Acq On : 18 Aug 2023 20:53
Operator : CG\JU
Sample : 04086-21
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB04

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-BF080123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134851.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.251	191	198	211	rVB	97975	182799	5.66%	0.919%
2	5.416	562	566	570	rBV	1566791	1372435	42.49%	6.902%
3	6.228	699	704	708	rBV	59186	49593	1.54%	0.249%
4	6.357	722	726	729	rBV	33808	32493	1.01%	0.163%
5	6.422	733	737	747	rBV	949712	835738	25.87%	4.203%
6	6.792	796	800	803	rBV	957198	759800	23.52%	3.821%
7	6.851	807	810	818	rVV	57213	50803	1.57%	0.255%
8	7.192	864	868	872	rVB	52774	44041	1.36%	0.221%
9	7.351	890	895	898	rBV	1995026	1949458	60.35%	9.804%
10	7.581	931	934	938	rBV2	20251	32662	1.01%	0.164%
11	8.069	1013	1017	1021	rVB	1256940	979724	30.33%	4.927%
12	8.292	1051	1055	1057	rBV	846449	636565	19.71%	3.201%
13	8.316	1057	1059	1066	rVB	936376	763621	23.64%	3.840%
14	8.428	1076	1078	1081	rBV	53396	47568	1.47%	0.239%
15	8.457	1081	1083	1088	rVB	66955	56514	1.75%	0.284%
16	8.869	1150	1153	1162	rVB	119760	115756	3.58%	0.582%
17	9.151	1196	1201	1204	rBV	3335851	3230277	100.00%	16.245%
18	9.269	1216	1221	1224	rBV	1523073	1345936	41.67%	6.769%
19	9.827	1311	1316	1319	rBV	1032430	958596	29.68%	4.821%
20	10.616	1446	1450	1453	rBV	1823425	1585027	49.07%	7.971%
21	11.316	1565	1569	1572	rBV	790692	711528	22.03%	3.578%
22	11.486	1584	1598	1616	rBV4	23183	131461	4.07%	0.661%
23	12.910	1836	1840	1843	rBV	3197019	2825883	87.48%	14.212%
24	13.962	2015	2019	2034	rBV	819406	723928	22.41%	3.641%
25	15.433	2264	2269	2275	rBV	356019	462087	14.30%	2.324%

Sum of corrected areas: 19884293

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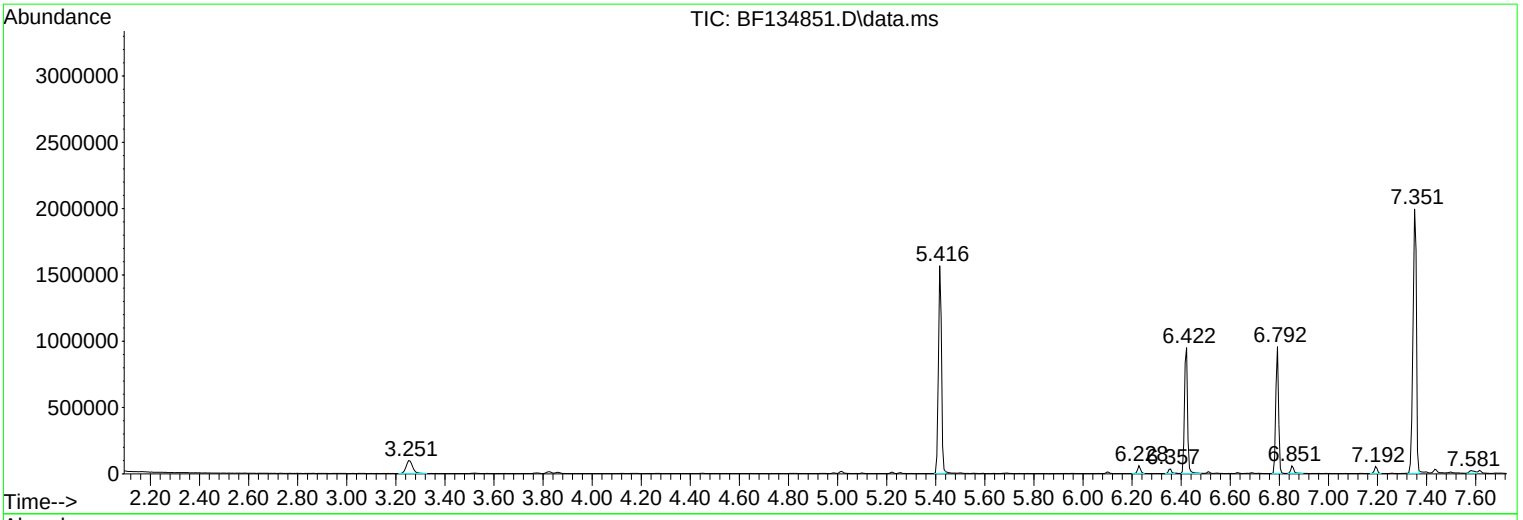
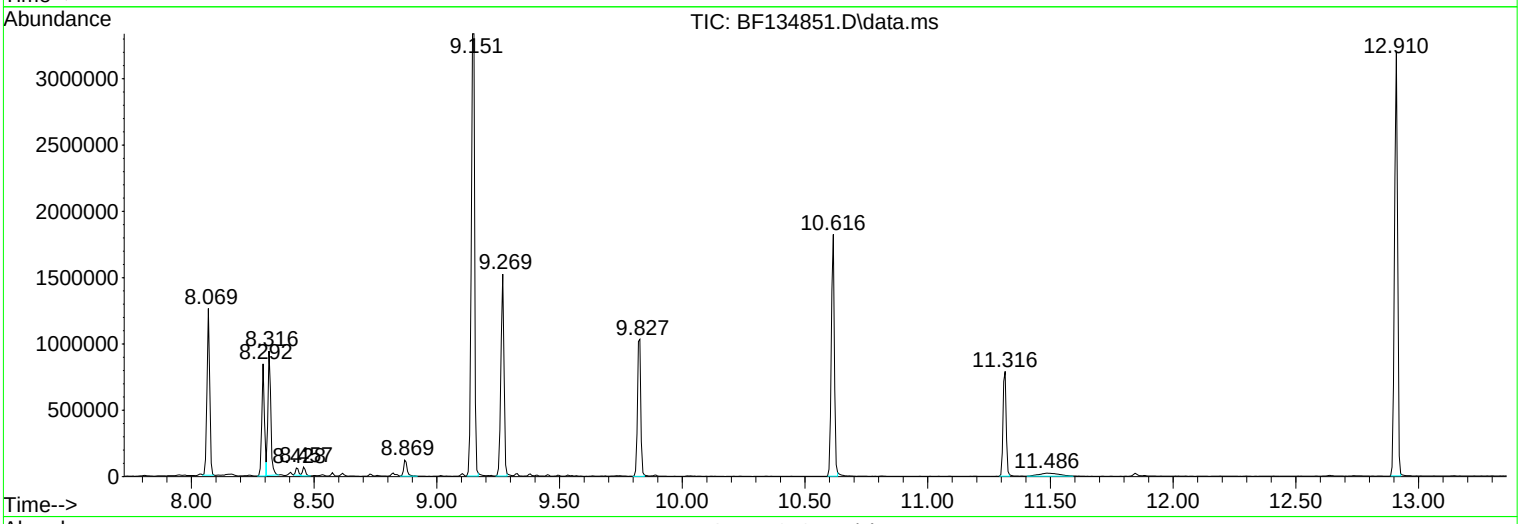
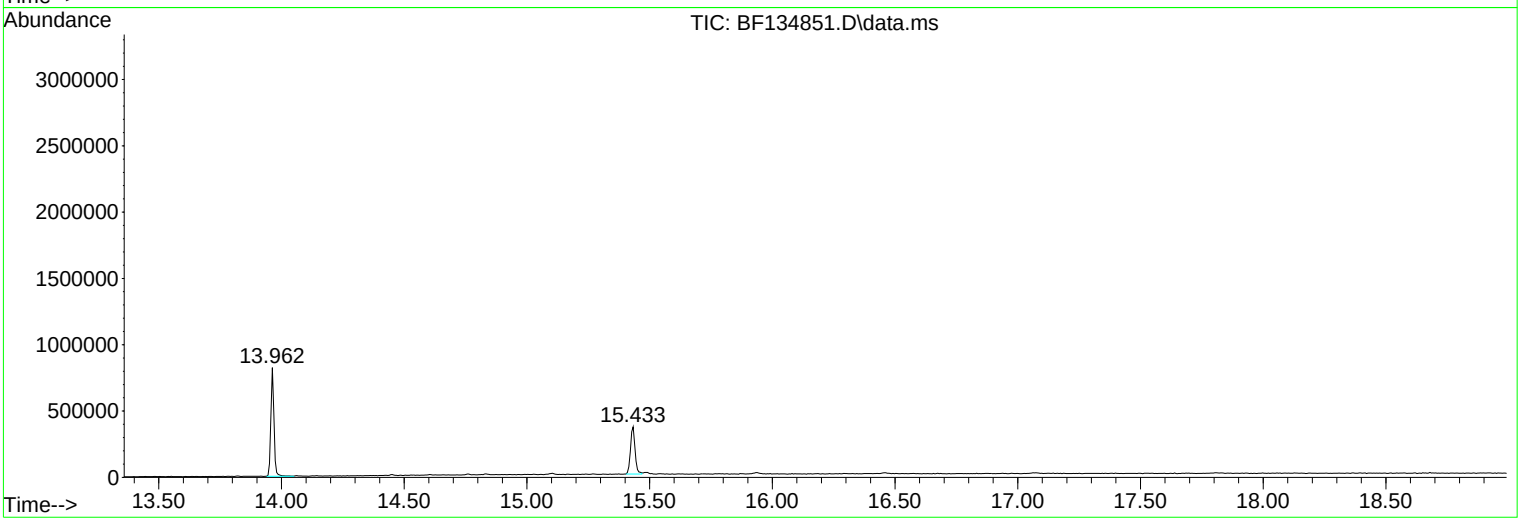
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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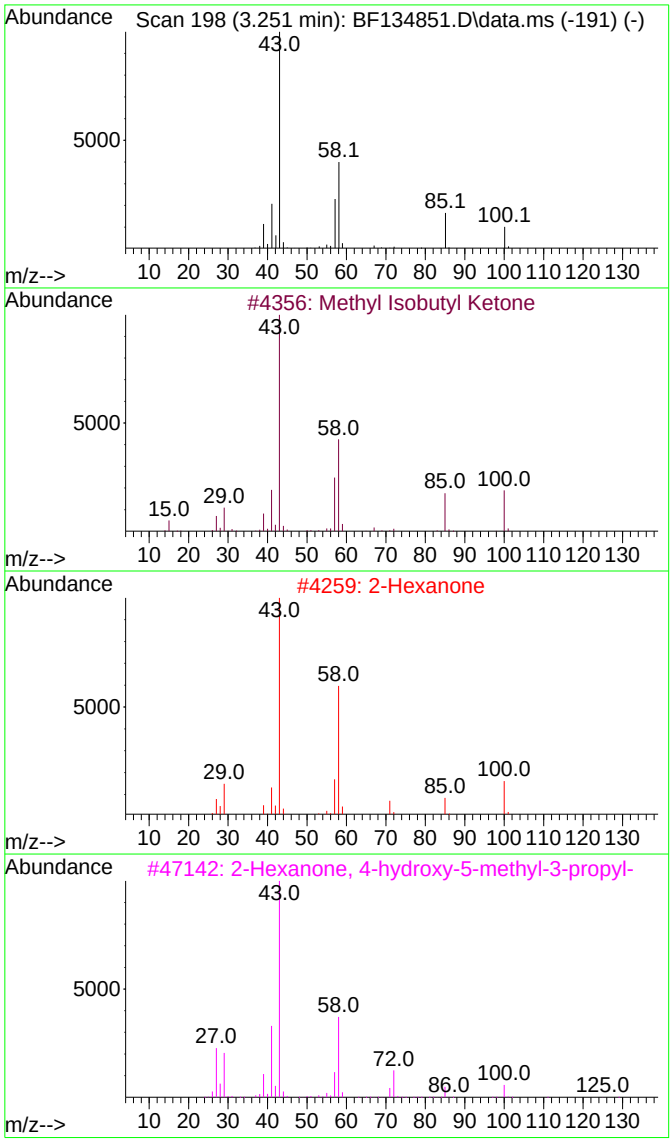
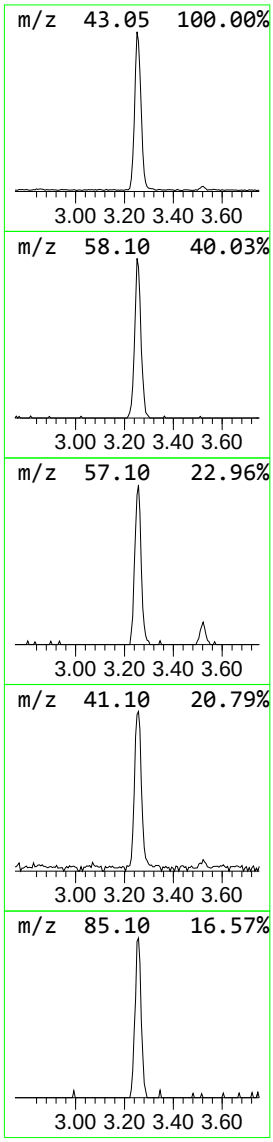
****
Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.251	4.81 ng	182799	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	86
2	2-Hexanone	100	C6H12O	000591-78-6	80
3	2-Hexanone, 4-hydroxy-5-methyl-3...	172	C10H20O2	061141-74-0	40
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	37
5	2,3-Pentanedione	100	C5H8O2	000600-14-6	14





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Instrument :
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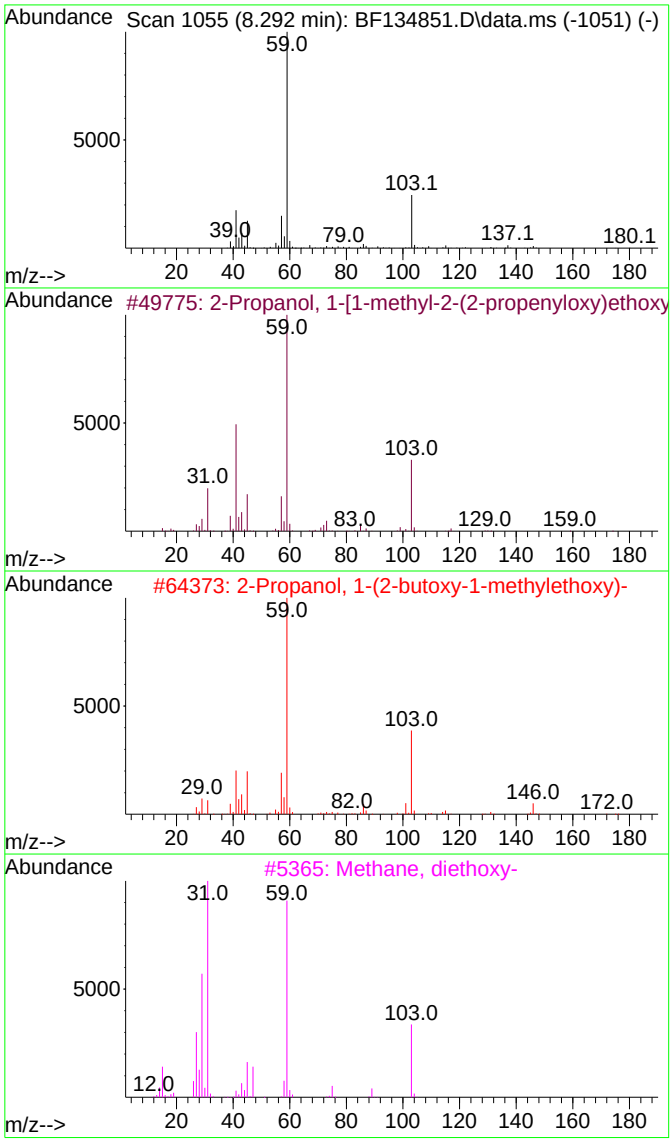
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

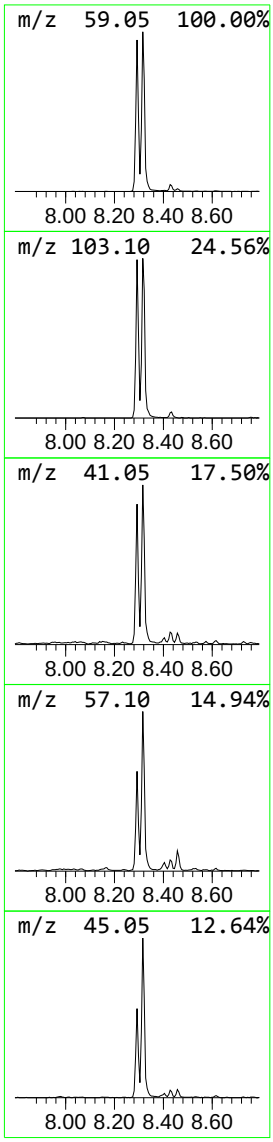
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.292	12.99 ng	636565	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	83
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
4	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	72
5	1-(1-Methoxypropan-2-yloxy)propa...	232	C12H24O4	1010367-13-4	64





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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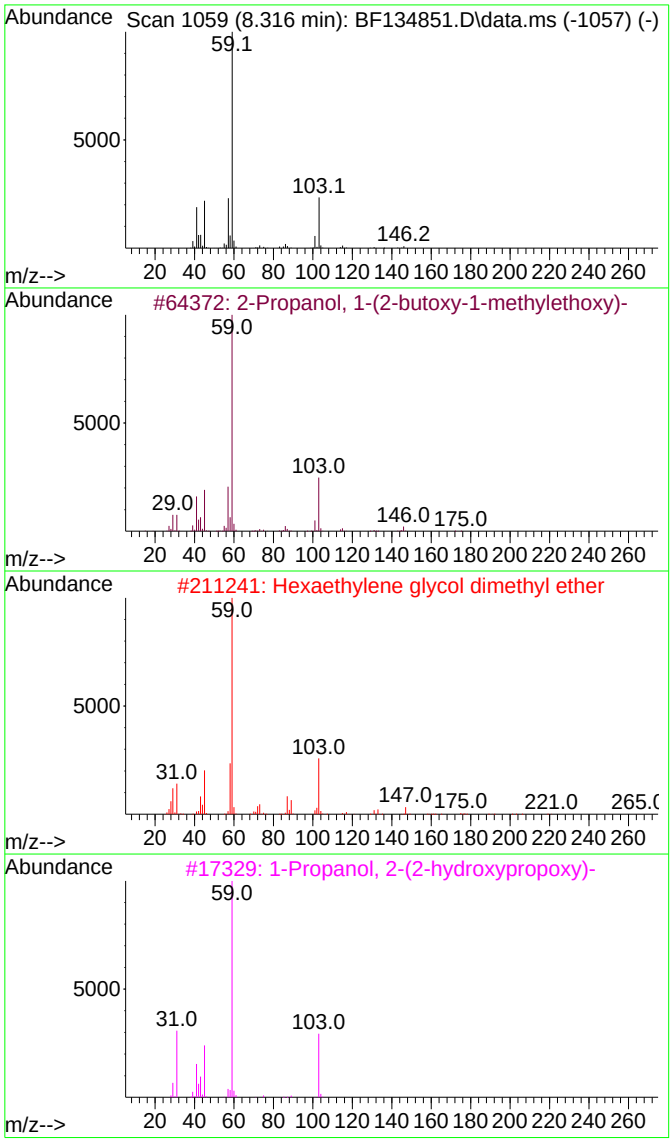
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

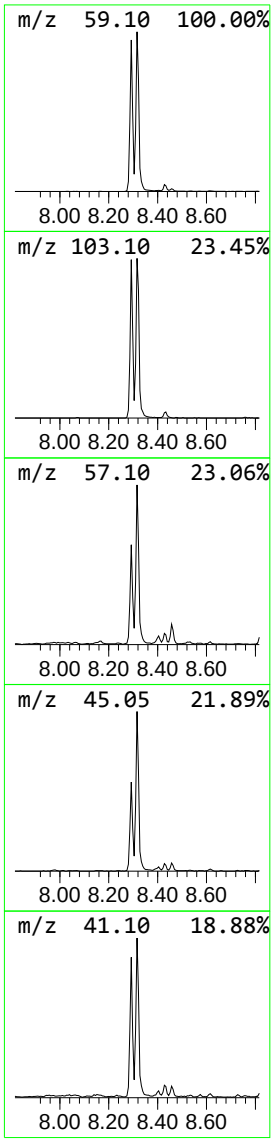
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.316	15.59 ng	763621	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90
2	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	78
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
4	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	72
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	72





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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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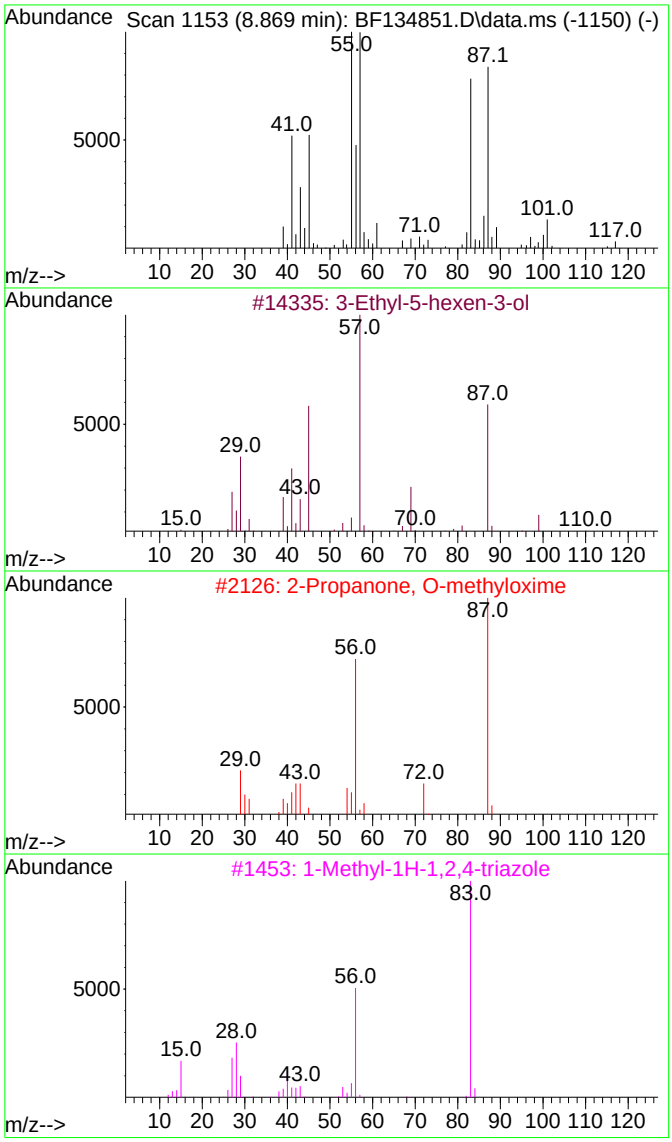
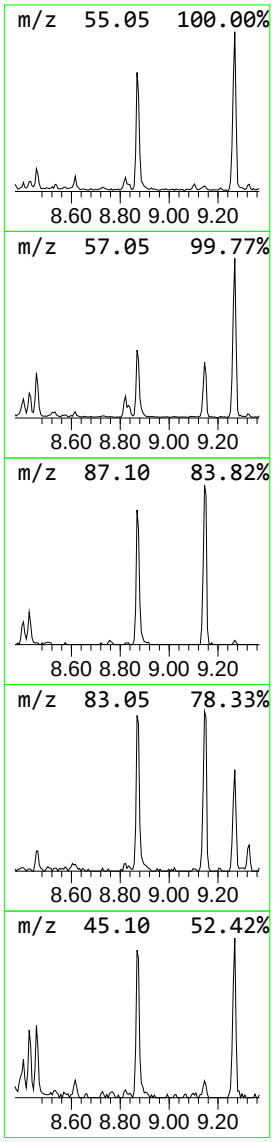
****

Peak Number 4 unknown8.869 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.869	2.36 ng	115756	Naphthalene-d8	8.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethyl-5-hexen-3-ol	128	C8H16O	001907-46-6	35
2	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	27
3	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	27
4	Cyclopropanecarboxylic acid, 1-a...	101	C4H7NO2	022059-21-8	27
5	3-Pentanol, 2,3,4-trimethyl-	130	C8H18O	003054-92-0	27





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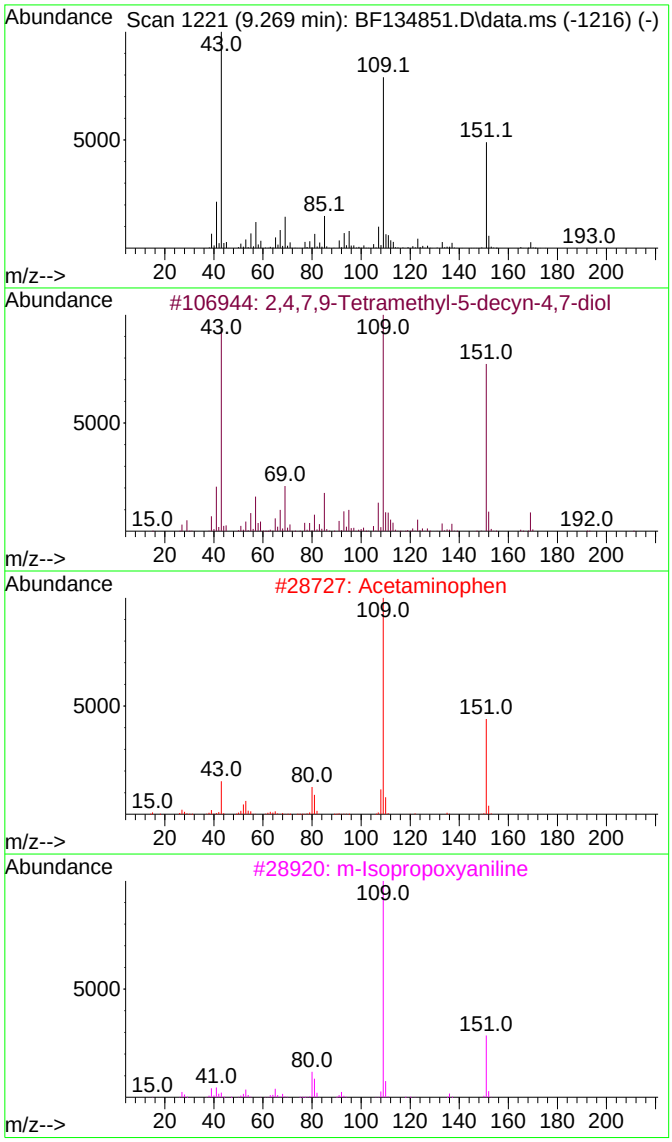
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

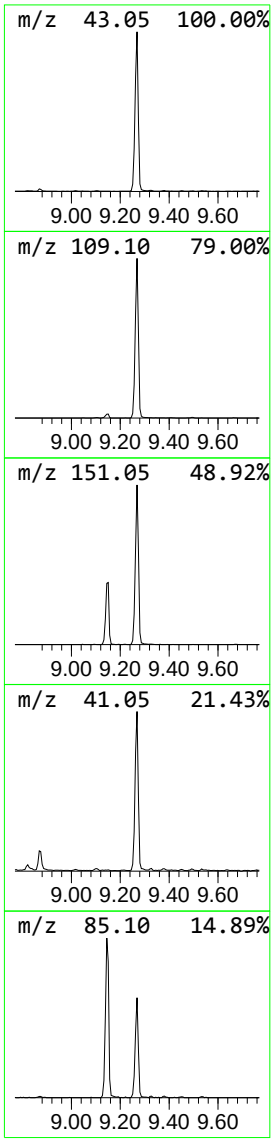
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.269	28.08 ng	1345940	Acenaphthene-d10	9.827

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Acetaminophen	151	C8H9NO2	000103-90-2	59
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
5	Metacetamol	151	C8H9NO2	000621-42-1	59





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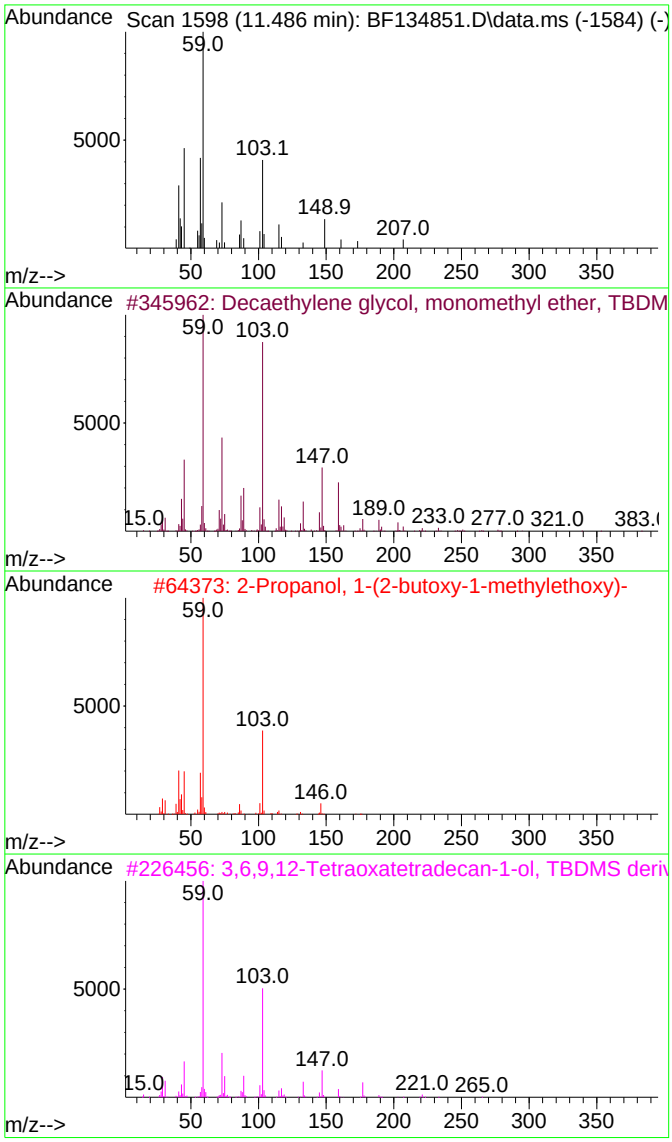
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

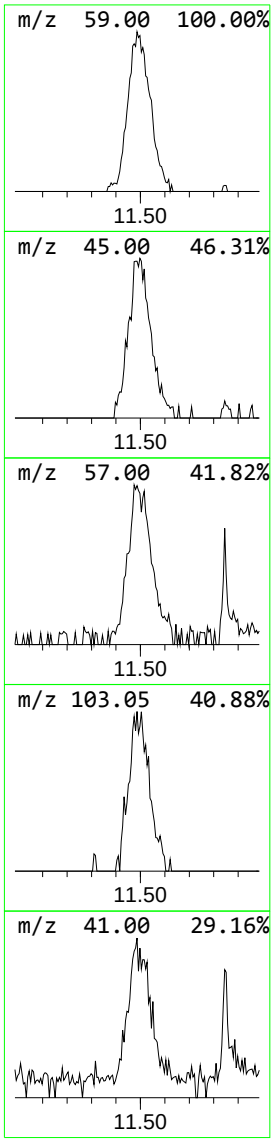
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Decaethylene glycol, monome... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.486	3.70 ng	131461	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decaethylene glycol, monomethyl ...	586	C27H58O11Si	1000352-12-0	50
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	50
3	3,6,9,12-Tetraoxatetradecan-1-ol...	322	C15H34O5Si	1000352-09-6	42
4	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	42
5	Ethyl 2,5,8,11,14,17-hexaoxanona...	338	C15H30O8	1000366-80-6	40





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
Methyl Isobutyl...	3.251	4.8	ng	182799	1	6.792	759800	20.0
2-Propanol, 1-[...	8.292	13.0	ng	636565	2	8.069	979724	20.0
2-Propanol, 1-(...	8.316	15.6	ng	763621	2	8.069	979724	20.0
unknown8.869	8.869	2.4	ng	115756	2	8.069	979724	20.0
2,4,7,9-Tetrame...	9.269	28.1	ng	1345940	3	9.827	958596	20.0
Decaethylene gl...	11.486	3.7	ng	131461	4	11.316	711528	20.0