LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131973.D
Acq On : 09 Jan 2023 20:33
Operator : CG\JU
Sample : 01045-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-TANK-11-12-31-32-33

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-BF010923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	487	492	500	rVB	305409	351038	10.77%	2.005%
2	5.392	558	562	573	rBV	1293952	1146900	35.20%	6.549%
3	6.416	733	736	748	rBV	860231	721500	22.15%	4.120%
4	6.781	795	798	802	rBV	524023	446654	13.71%	2.551%
5	7.357	890	896	899	rBV	1657973	1739683	53.40%	9.935%
6	8.075	1013	1018	1021	rBV	650044	558721	17.15%	3.191%
7	8.298	1051	1056	1058	rBV	596451	589841	18.10%	3.368%
8	8.322	1058	1060	1070	rVB	656969	510960	15.68%	2.918%
9	8.410	1070	1075	1077	rBV	170824	138918	4.26%	0.793%
10	9.157	1196	1202	1205	rBV	3733698	3258018	100.00%	18.605%
11	9.833	1313	1317	1320	rBV	843129	664103	20.38%	3.792%
12	10.551	1436	1439	1443	rBV	52656	49984	1.53%	0.285%
13	10.627	1448	1452	1456	rBV	2002863	1974443	60.60%	11.275%
14	11.327	1567	1571	1574	rVB	784437	701721	21.54%	4.007%
15	11.886	1663	1666	1670	rVB	425146	374714	11.50%	2.140%
16	12.921	1837	1842	1845	rBV	3275895	2925988	89.81%	16.709%
17	13.815	1991	1994	2003	rVB	97724	135135	4.15%	0.772%
18	13.974	2017	2021	2025	rVB	484956	414461	12.72%	2.367%
19	14.598	2124	2127	2133	rVB	463666	436879	13.41%	2.495%
20	15.439	2265	2270	2276	rBV	314965	371622	11.41%	2.122%

Sum of corrected areas: 17511283

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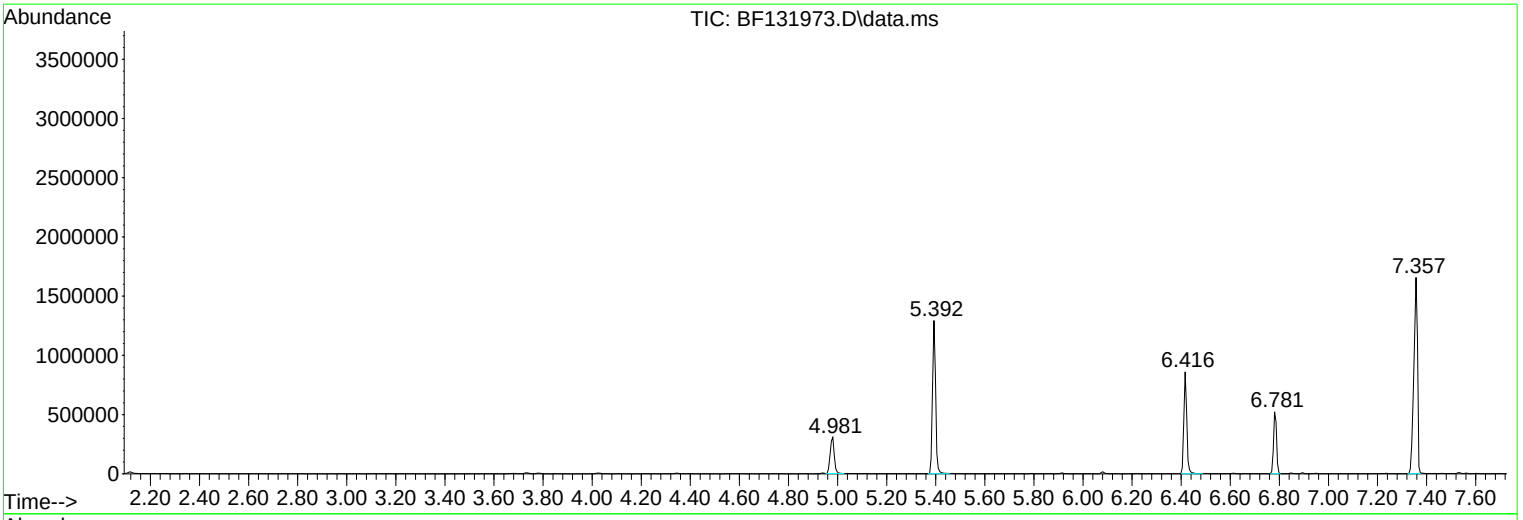
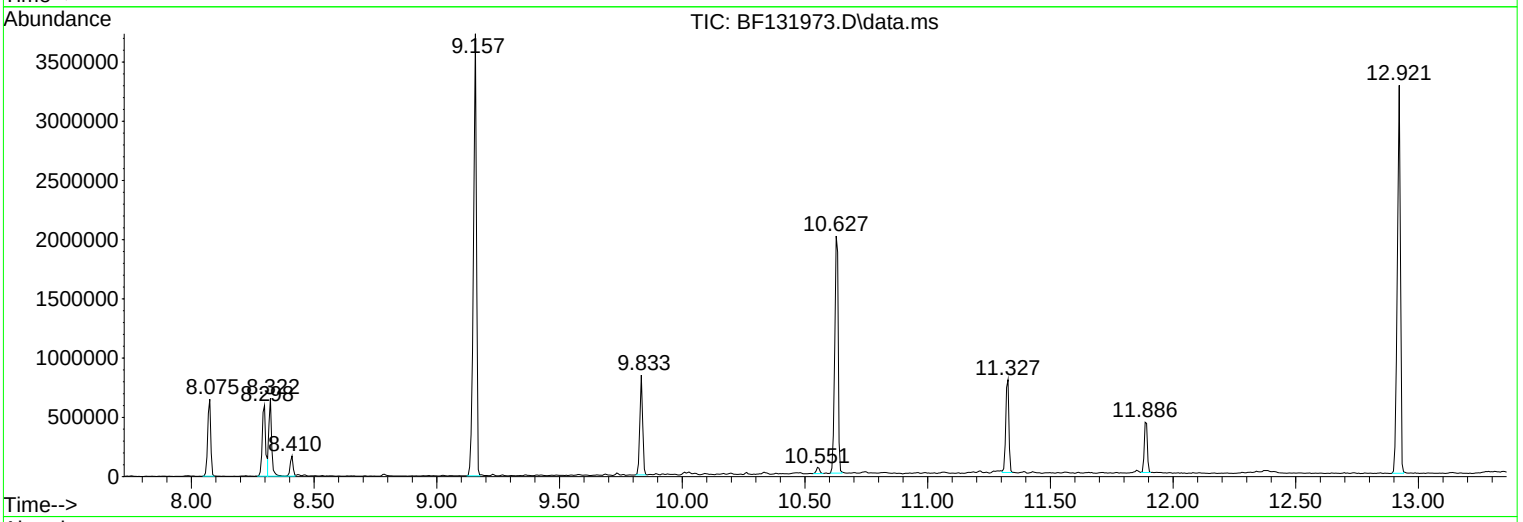
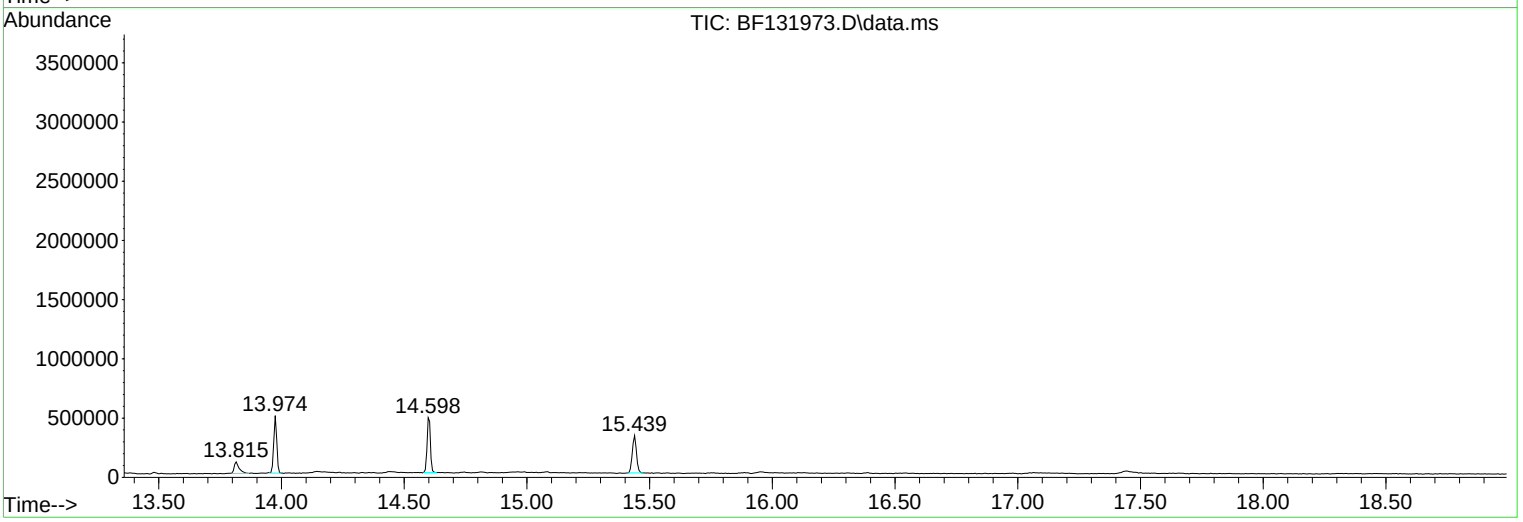
Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-TANK-11-12-31-32-33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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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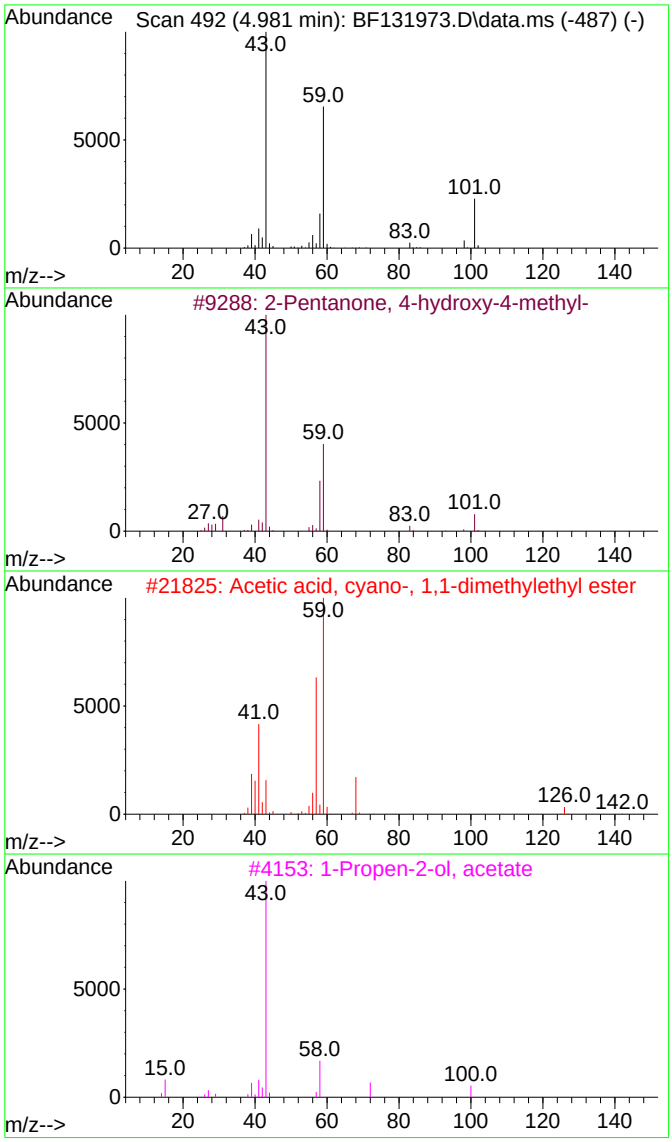
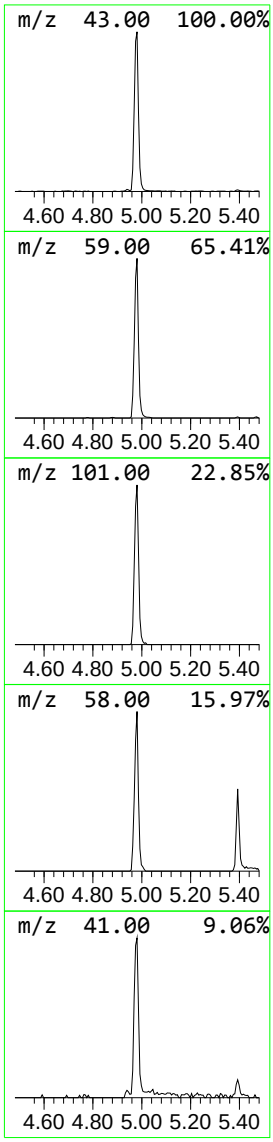
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	15.72 ng	351038	1,4-Dichlorobenzene-d4	6.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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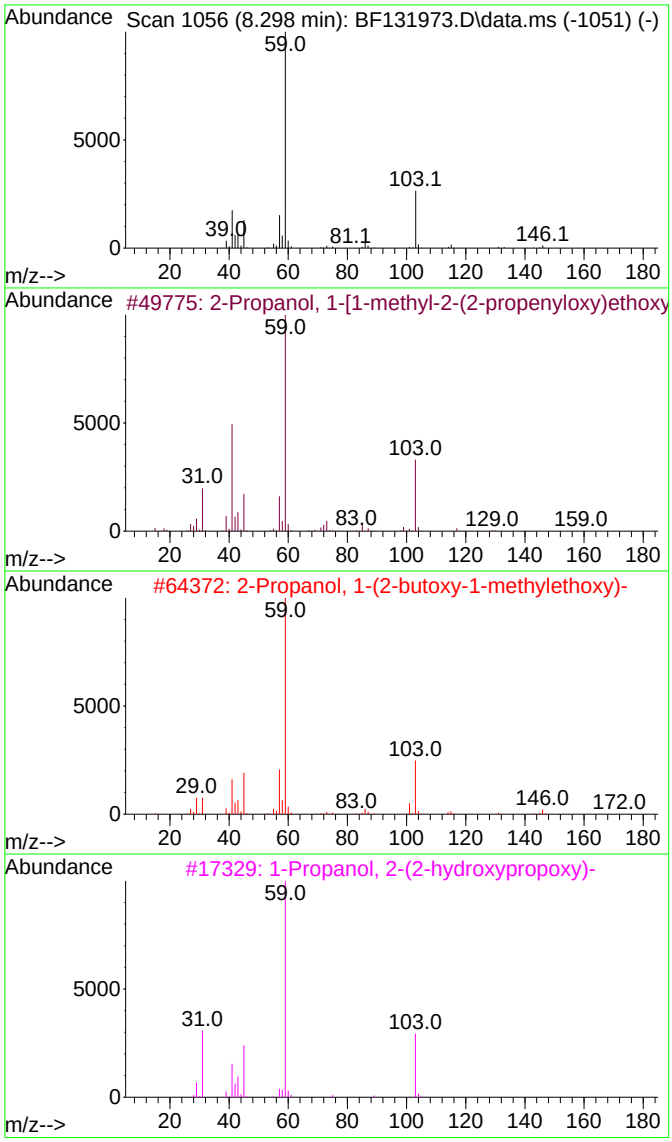
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

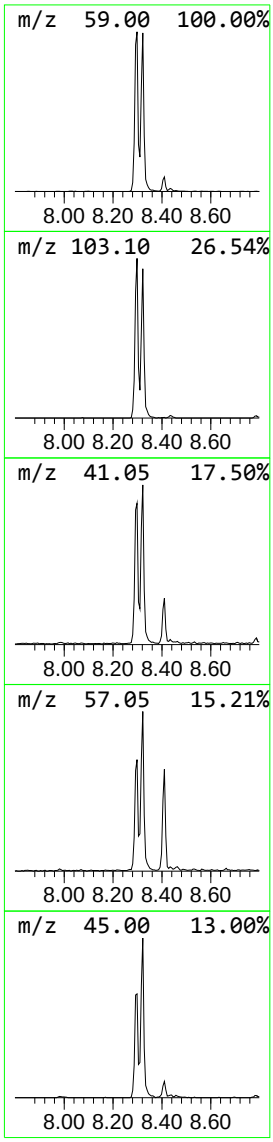
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.298	21.11 ng	589841	Naphthalene-d8	8.075

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	83
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
4	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64
5	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64





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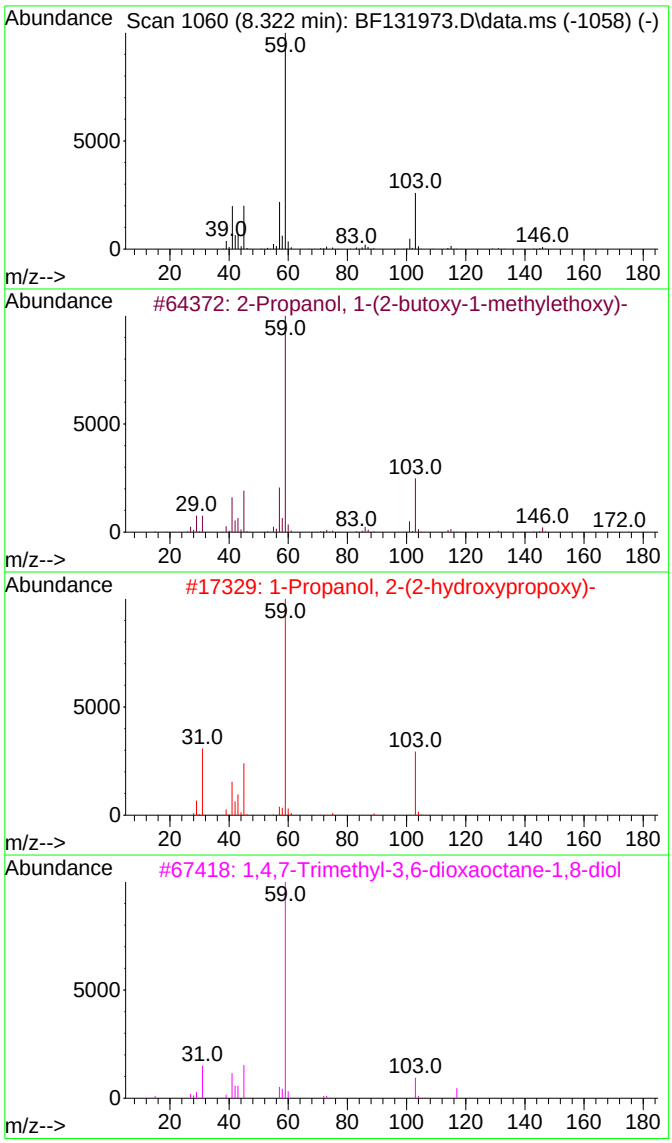
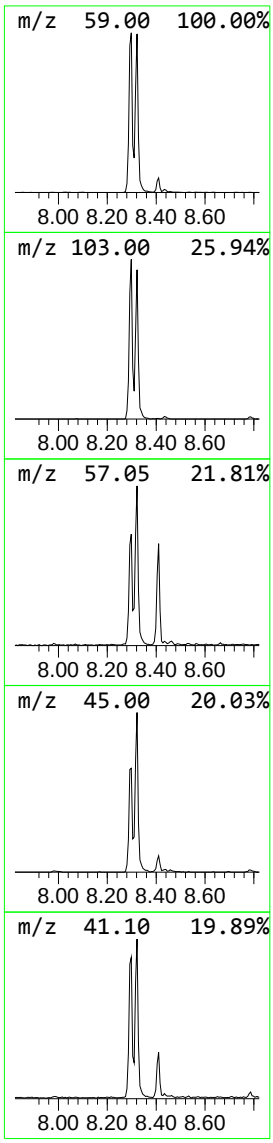
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.322	18.29 ng	510960	Naphthalene-d8	8.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
3	1,4,7-Trimethyl-3,6-dioxaoctane-...	192	C9H20O4	1000423-63-2	72
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
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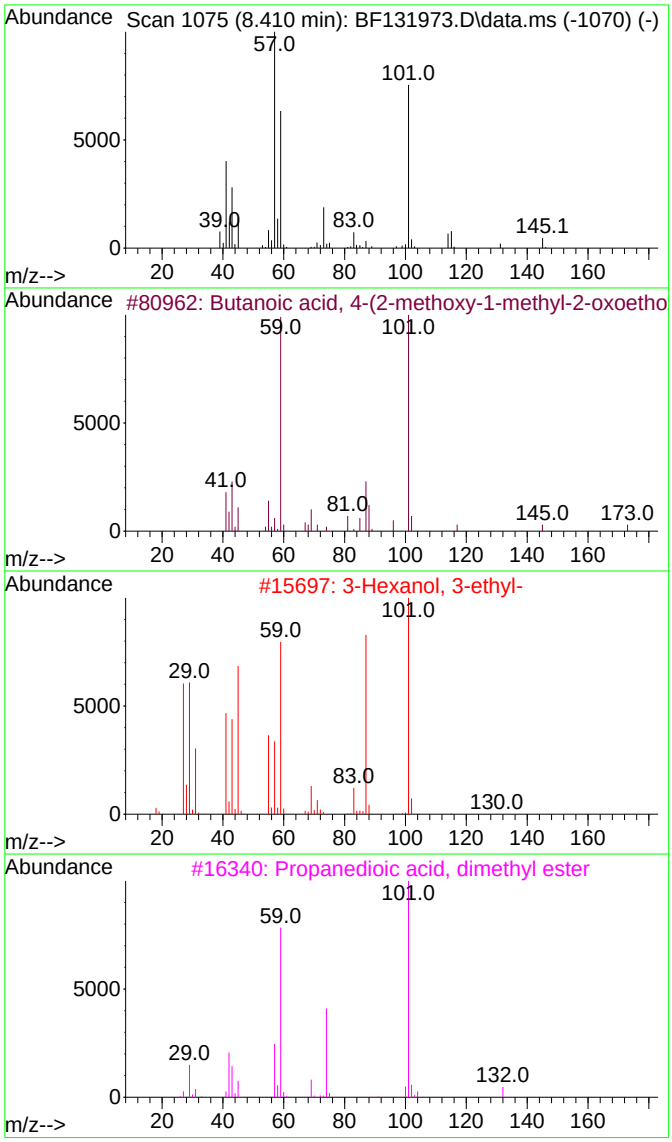
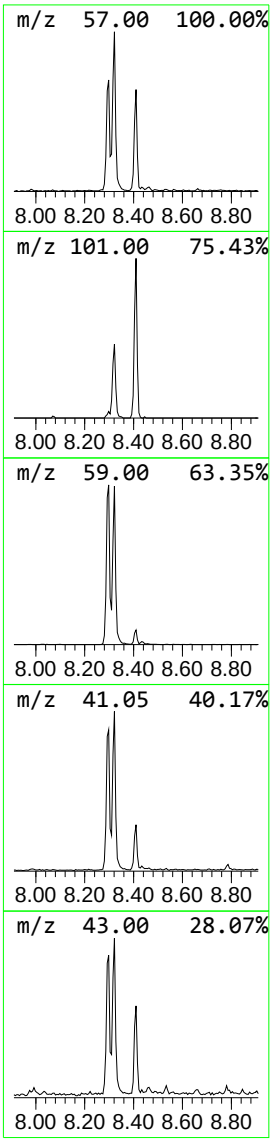
****
Peak Number 4 Butanoic acid, 4-(2-methoxy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.410	4.97 ng	138918	Naphthalene-d8	8.075

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	50
2	3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	50
3	Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	38
4	Butanedioic acid, monomethyl ester	132	C5H8O4	003878-55-5	38
5	Adipic acid, di(4-methoxy-2-meth...	346	C18H34O6	1000324-30-7	37





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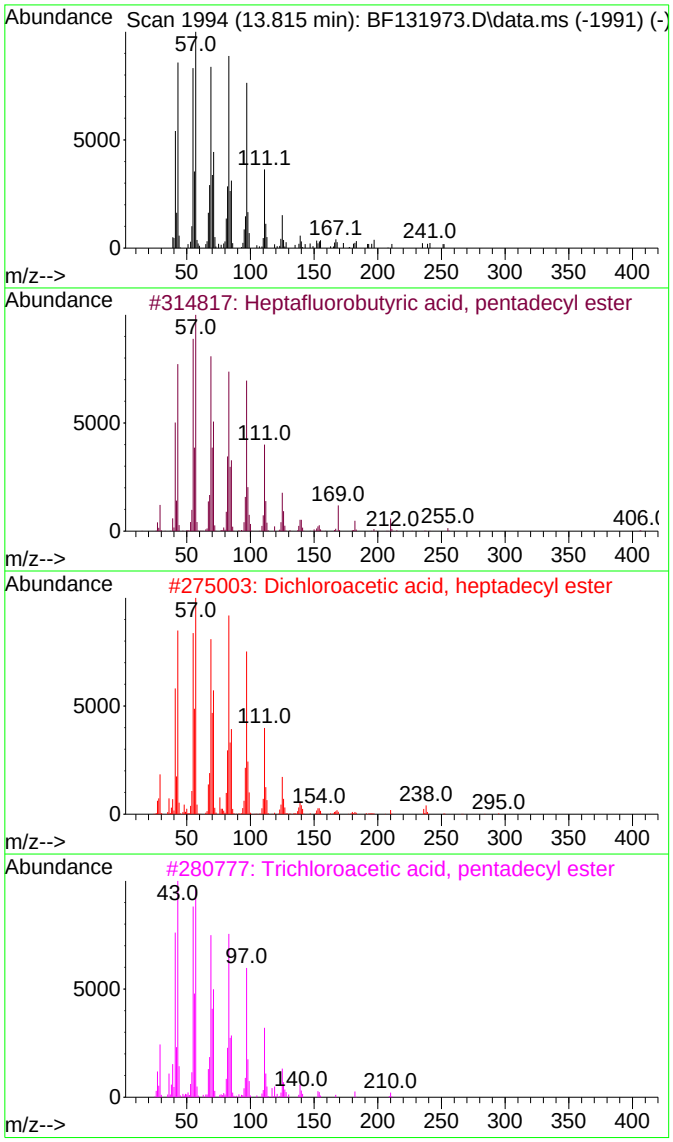
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

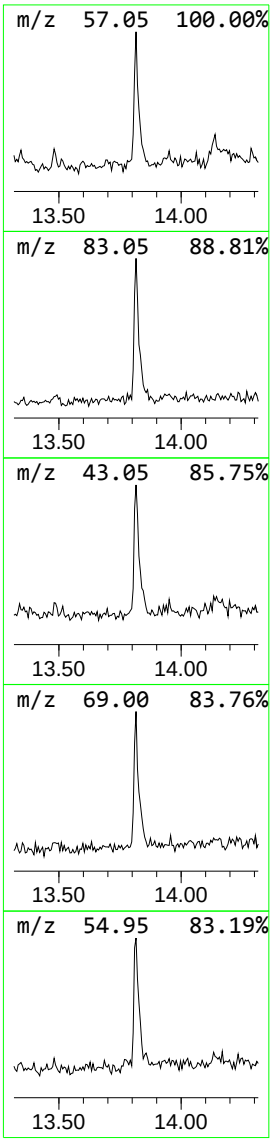
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	6.52 ng	135135	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





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Instrument :
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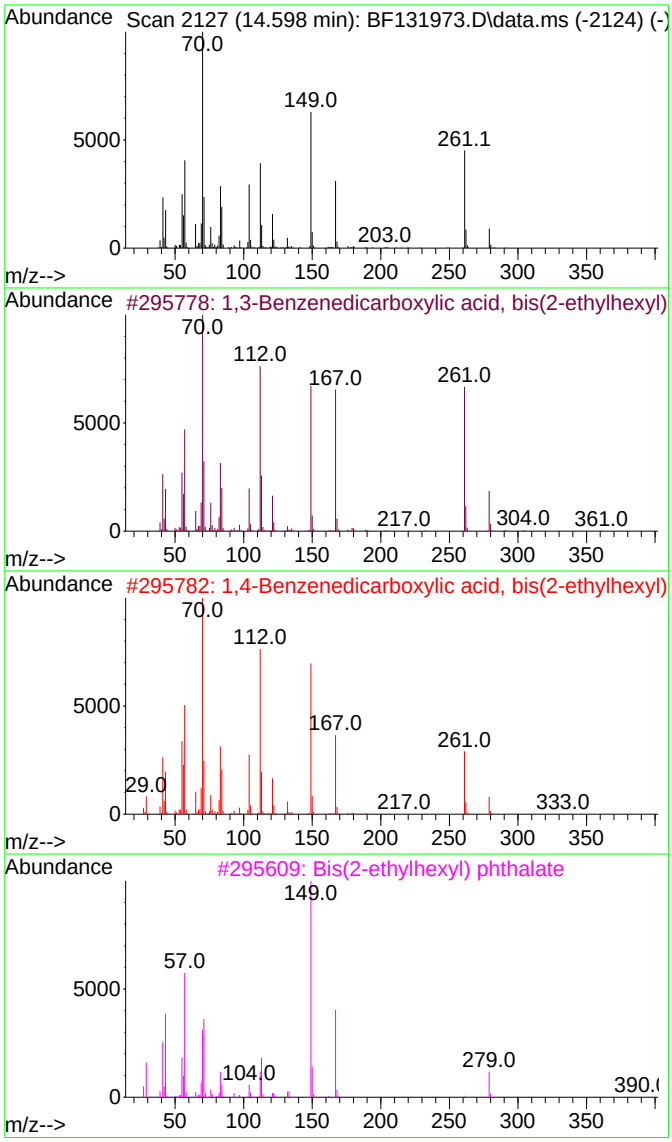
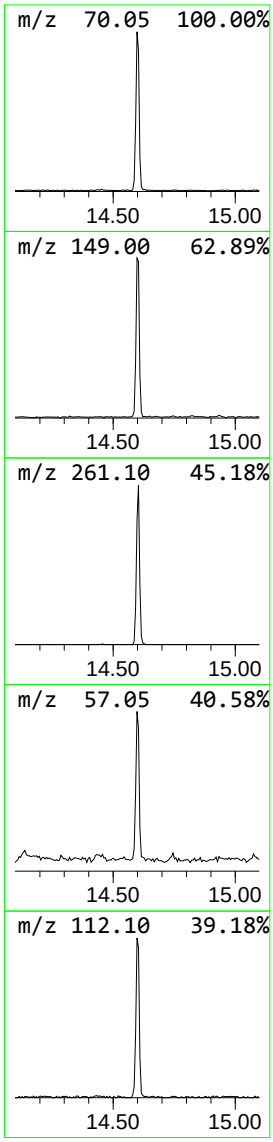
****

Peak Number 6 unknown14.598 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	21.08 ng	436879	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	47
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	46
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	25
4	Cyclohexaneamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	25
5	Phthalic acid, 3,5-difluoropheny...	390	C22H24F2O4	1000315-51-3	22





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-...	4.981	15.7	ng	351038	1	6.781	446654	20.0
2-Propanol, 1-[...	8.298	21.1	ng	589841	2	8.075	558721	20.0
2-Propanol, 1-(...	8.322	18.3	ng	510960	2	8.075	558721	20.0
Butanoic acid, ...	8.410	5.0	ng	138918	2	8.075	558721	20.0
Heptafluorobuty...	13.815	6.5	ng	135135	5	13.974	414461	20.0
unknown14.598	14.598	21.1	ng	436879	5	13.974	414461	20.0