LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071024\
Data File : BF138504.D
Acq On : 10 Jul 2024 16:39
Operator : CG\JU
Sample : P3190-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
240702108-05

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-BF070924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138504.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	15	19	rBV	4143703	5824936	100.00%	29.420%
2	5.075	505	508	514	rVB	142507	143760	2.47%	0.726%
3	5.486	574	578	582	rBV	1135681	970305	16.66%	4.901%
4	6.492	745	749	757	rVB	814071	681302	11.70%	3.441%
5	6.863	808	812	815	rBV	688879	534288	9.17%	2.699%
6	7.427	902	908	911	rBV	1650538	1584375	27.20%	8.002%
7	7.675	946	950	954	rBV	110697	88490	1.52%	0.447%
8	8.145	1025	1030	1033	rBV	834761	706648	12.13%	3.569%
9	8.451	1079	1082	1094	rBV	157512	167279	2.87%	0.845%
10	9.221	1207	1213	1216	rBV	2921702	2694503	46.26%	13.609%
11	9.898	1323	1328	1331	rBV	944287	749327	12.86%	3.785%
12	10.686	1458	1462	1465	rBV	1280915	1094242	18.79%	5.527%
13	11.380	1576	1580	1584	rBV	793866	662262	11.37%	3.345%
14	11.551	1606	1609	1613	rVB	64957	65584	1.13%	0.331%
15	11.904	1666	1669	1678	rBV2	212291	314497	5.40%	1.588%
16	12.686	1799	1802	1809	rBV	43009	60231	1.03%	0.304%
17	12.968	1845	1850	1853	rBV	2445813	2133404	36.63%	10.775%
18	13.862	1998	2002	2014	rBV	239013	317969	5.46%	1.606%
19	14.015	2024	2028	2032	rBV	489768	442801	7.60%	2.236%
20	15.480	2272	2277	2286	rBV	372346	469423	8.06%	2.371%
21	16.003	2362	2366	2374	rBV3	40906	93706	1.61%	0.473%

Sum of corrected areas: 19799332

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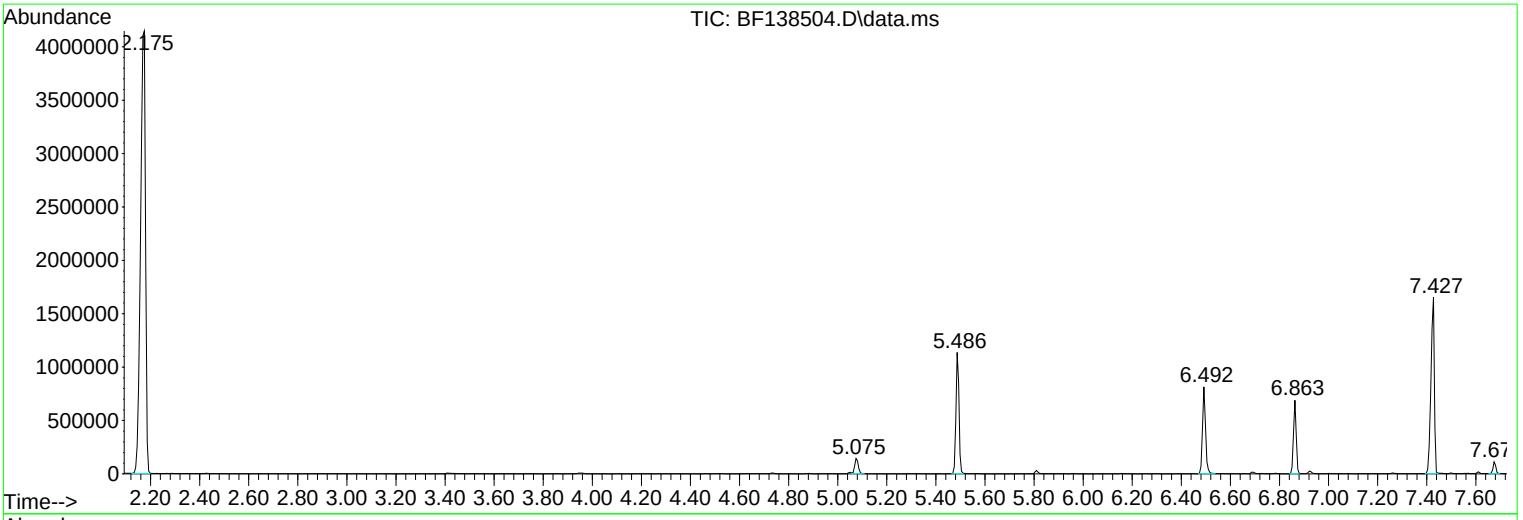
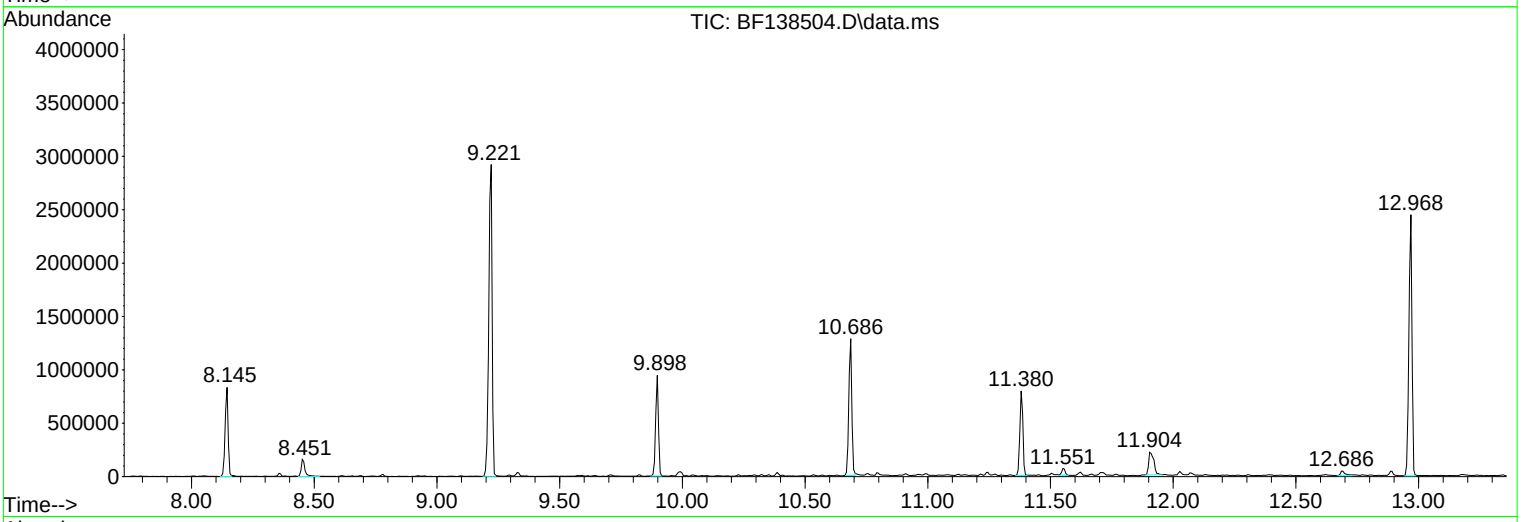
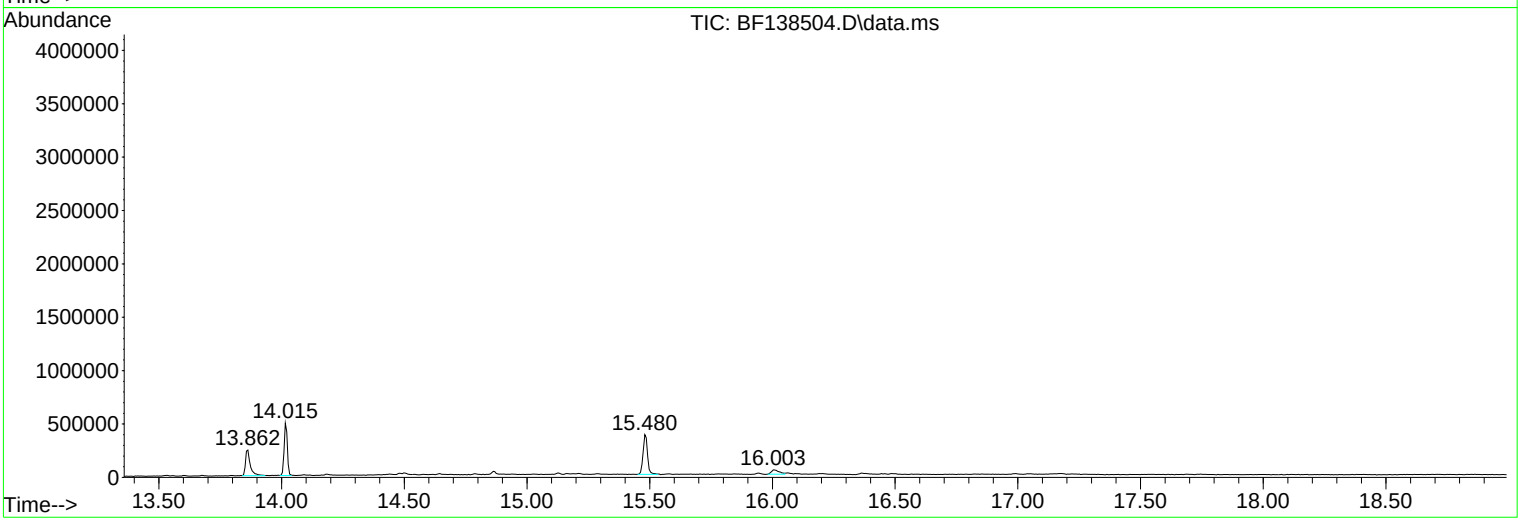
ClientSampleId :
240702108-05

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.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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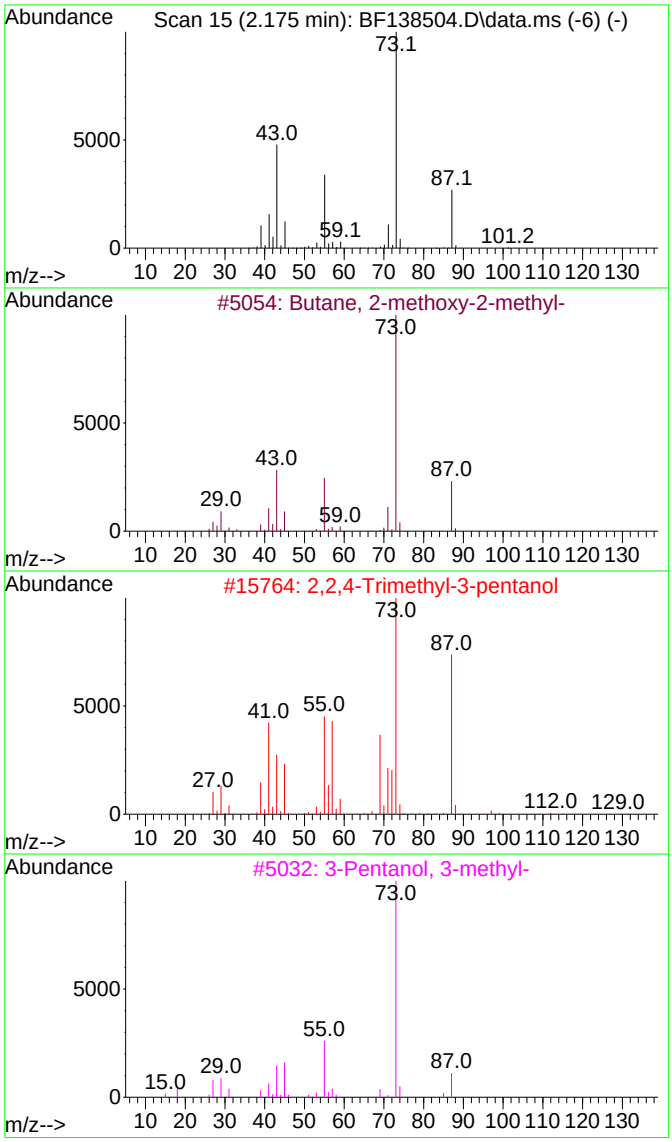
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

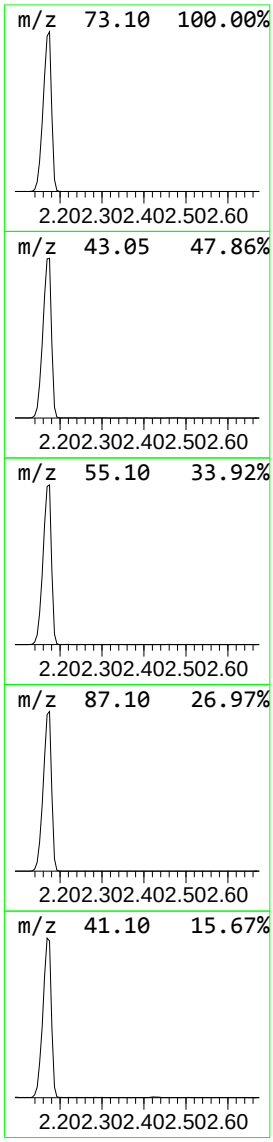
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	218.04 ng	5824940	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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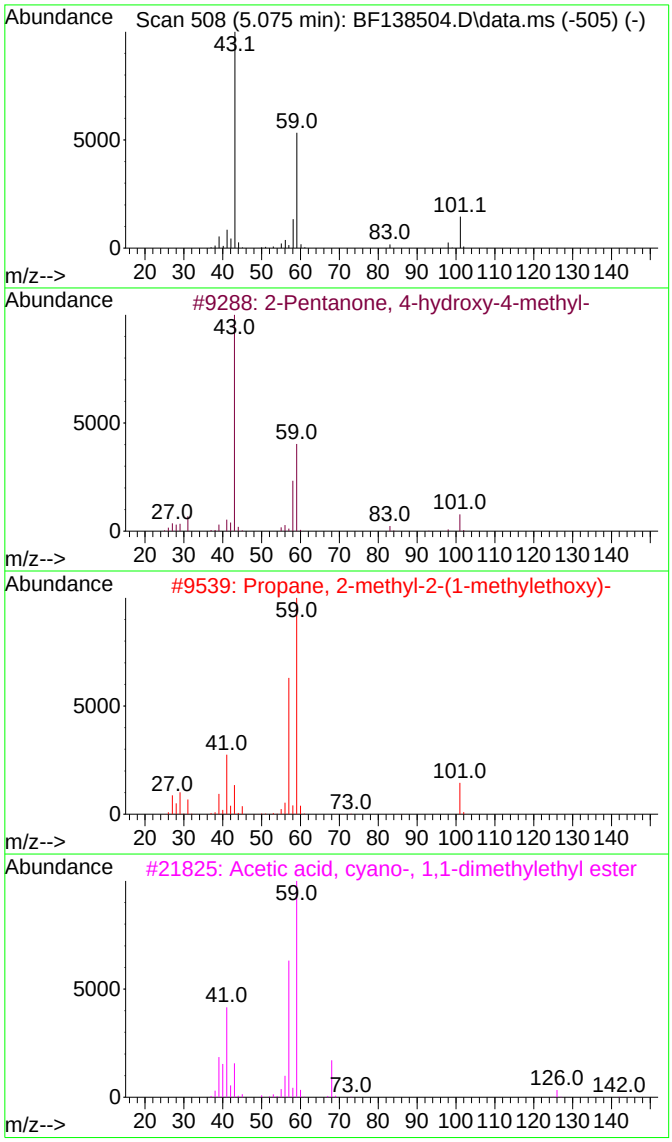
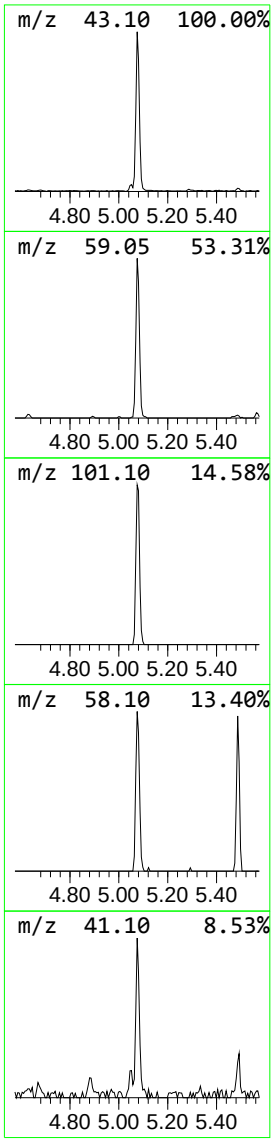
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.38 ng	143760	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF070924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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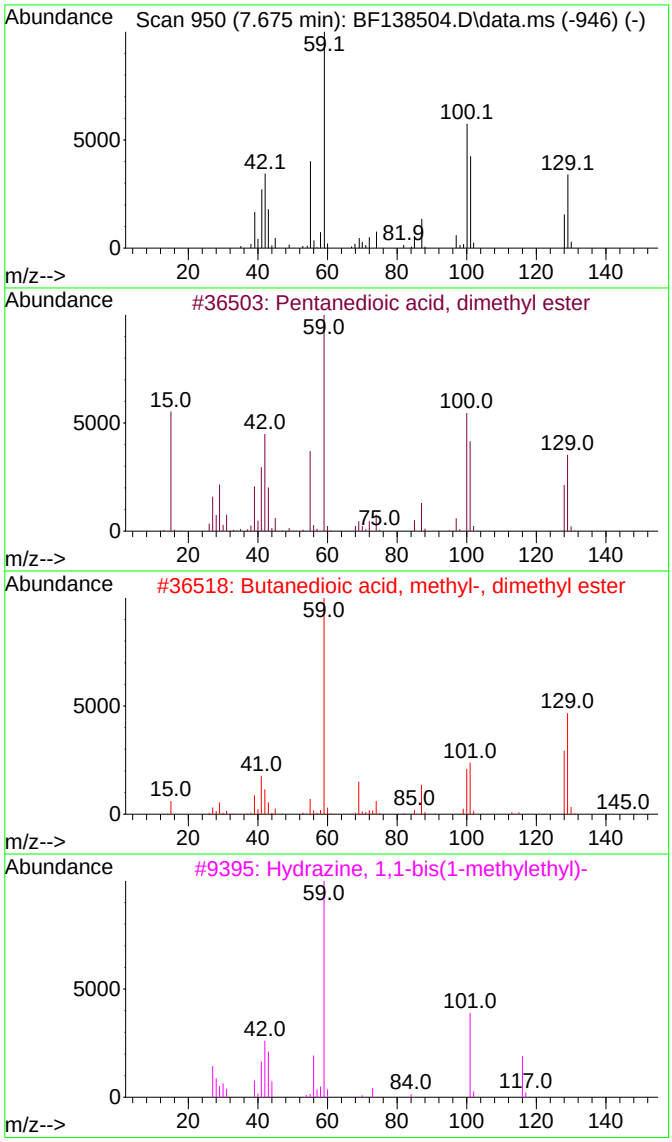
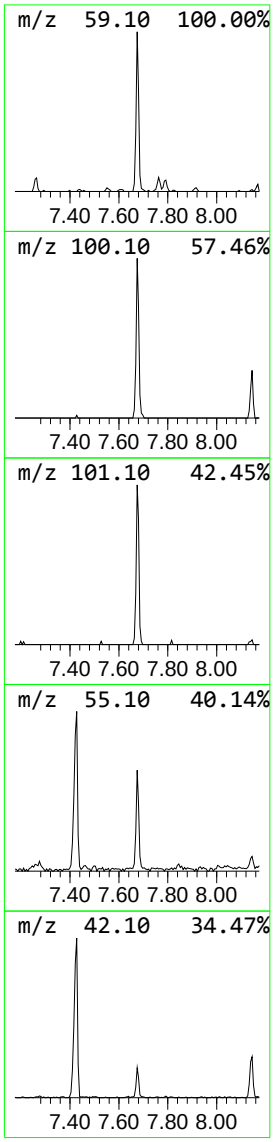
Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.675	2.50 ng	88490	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	42
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	28
5	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	25





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240702108-05

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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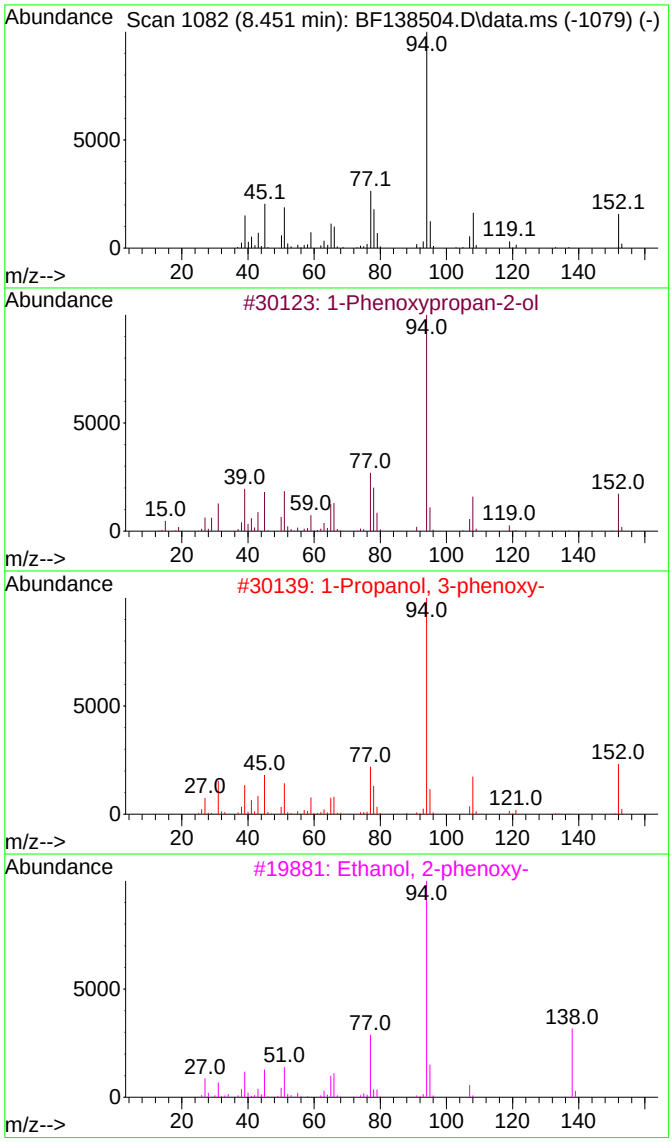
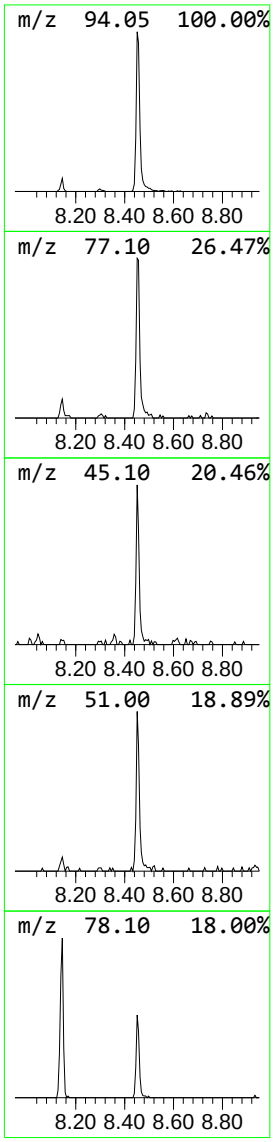
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	4.73 ng	167279	Naphthalene-d8	8.145

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	74
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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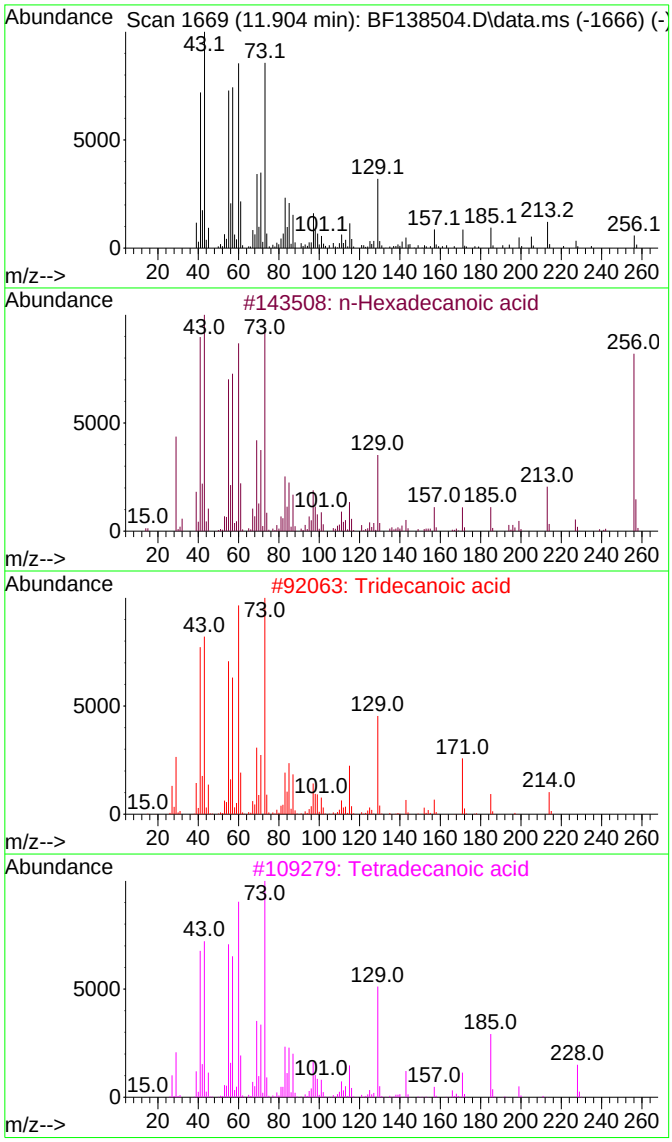
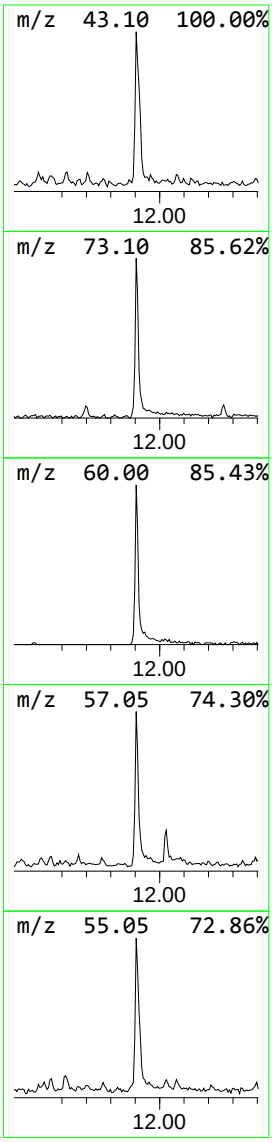
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	9.50 ng	314497	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





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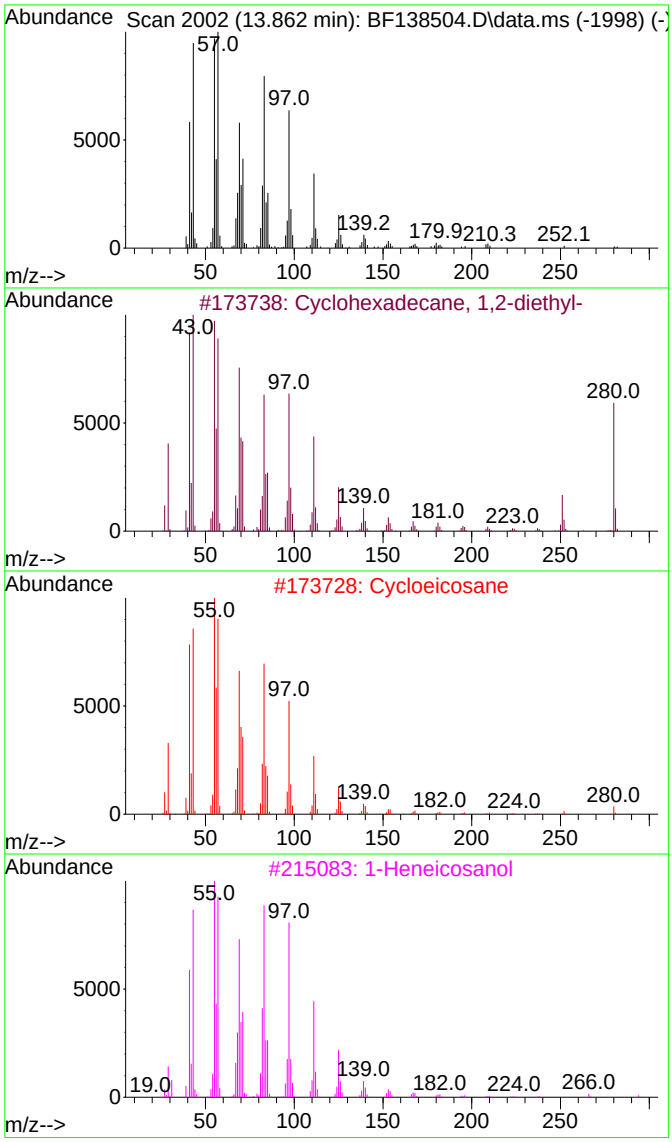
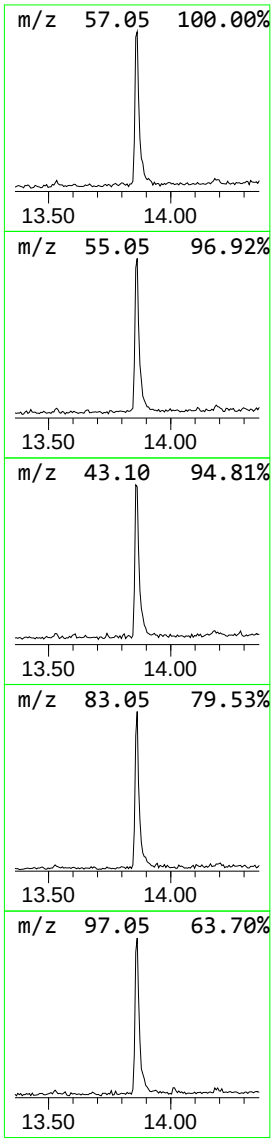
****

Peak Number 6 Cyclohexadecane, 1,2-diethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.862	14.36 ng	317969	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	97
2	Cycloeicosane	280	C20H40	000296-56-0	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5	1-Hexacosene	364	C26H52	018835-33-1	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

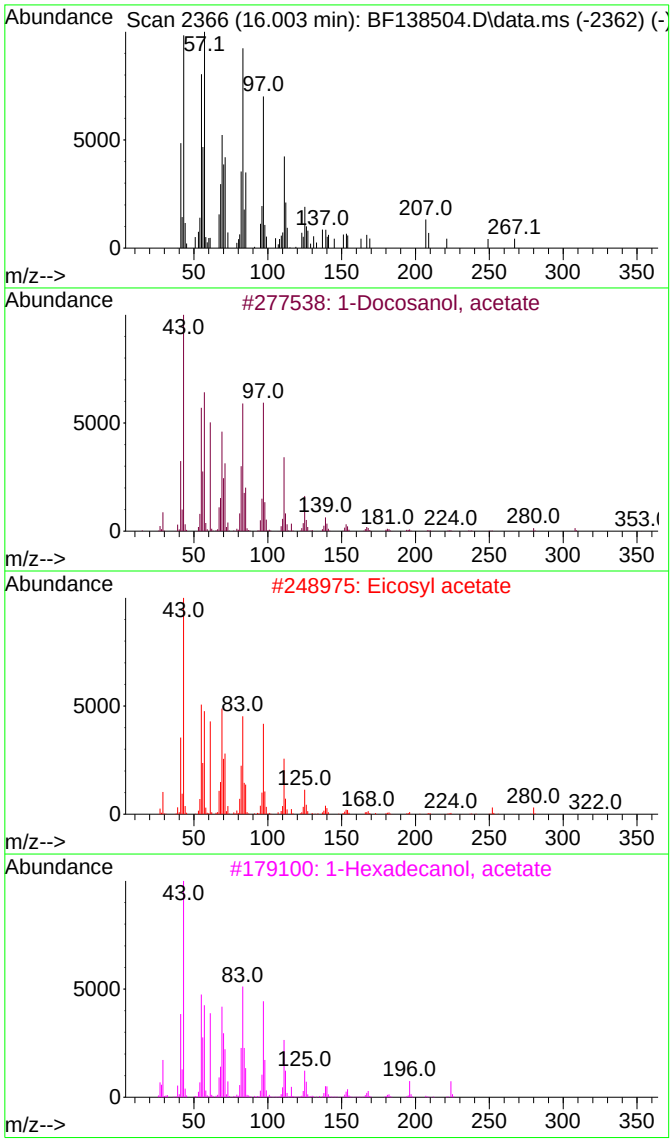
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

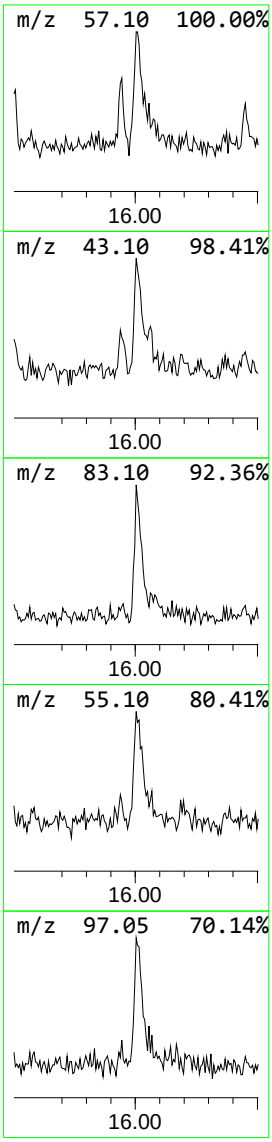
****

Peak Number 7 1-Docosanol, acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.003	3.99 ng	93706	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanol, acetate	368	C24H48O2	000822-26-4	91
2	Eicosyl acetate	340	C22H44O2	000822-24-2	91
3	1-Hexadecanol, acetate	284	C18H36O2	000629-70-9	91
4	Hexacosyl acetate	424	C28H56O2	000822-32-2	87
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	87





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
Butane, 2-metho...	2.175	218.0	ng	5824940	1	6.863	534288	20.0
2-Pentanone, 4-...	5.075	5.4	ng	143760	1	6.863	534288	20.0
Pentanedioic ac...	7.675	2.5	ng	88490	2	8.145	706648	20.0
1-Phenoxypropan...	8.451	4.7	ng	167279	2	8.145	706648	20.0
n-Hexadecanoic ...	11.904	9.5	ng	314497	4	11.380	662262	20.0
Cyclohexadecane...	13.862	14.4	ng	317969	5	14.015	442801	20.0
1-Docosanol, ac...	16.003	4.0	ng	93706	6	15.480	469423	20.0