LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062323\
Data File : BF133935.D
Acq On : 23 Jun 2023 10:54
Operator : CG\JU
Sample : 03274-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-1

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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133935.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	9	16	22	rVB	2931040	4164887	16.87%	6.419%
2	5.098	508	512	521	rVB	299520	351726	1.42%	0.542%
3	5.498	575	580	583	rBV	1930564	1886336	7.64%	2.907%
4	6.493	744	749	760	rVB	1593716	1542190	6.24%	2.377%
5	6.857	808	811	815	rBV	764999	609473	2.47%	0.939%
6	7.422	898	907	910	rBV	1951990	1979858	8.02%	3.051%
7	8.139	1025	1029	1032	rBV	1024405	811420	3.29%	1.251%
8	9.222	1207	1213	1216	rBV	3759272	3544026	14.35%	5.462%
9	9.898	1324	1328	1331	rBV	1143859	912118	3.69%	1.406%
10	9.975	1331	1341	1344	rVV	1971704	4201376	17.01%	6.475%
11	10.692	1457	1463	1467	rBV	2594621	2608027	10.56%	4.020%
12	11.392	1578	1582	1585	rBV	1204053	991565	4.02%	1.528%
13	11.927	1666	1673	1681	rBV	1034934	1178136	4.77%	1.816%
14	12.716	1802	1807	1815	rBV	763254	818597	3.31%	1.262%
15	12.992	1849	1854	1857	rBV	3936411	3914161	15.85%	6.033%
16	13.845	1987	1999	2003	rBV	2864303	7522705	30.46%	11.594%
17	13.945	2003	2016	2018	rVV2	8005085	24695405	100.00%	38.062%
18	13.968	2018	2020	2027	rVB	1706244	1571303	6.36%	2.422%
19	14.063	2032	2036	2040	rBV	902839	899033	3.64%	1.386%
20	15.557	2285	2290	2296	rBV	465628	680104	2.75%	1.048%

Sum of corrected areas: 64882446

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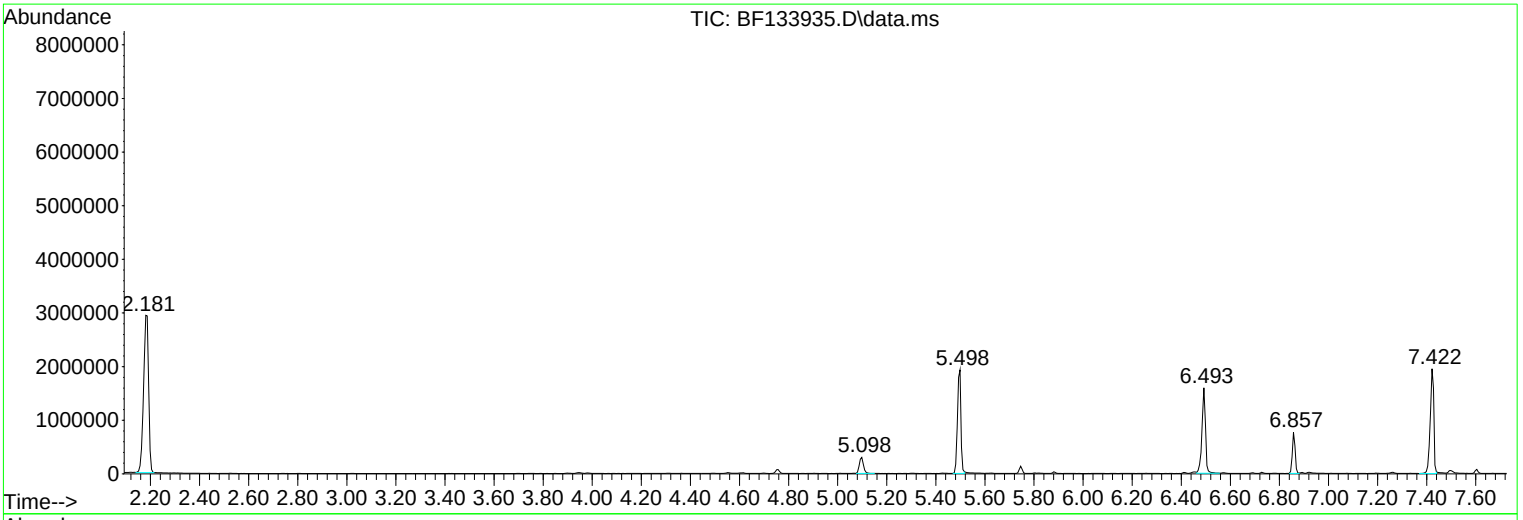
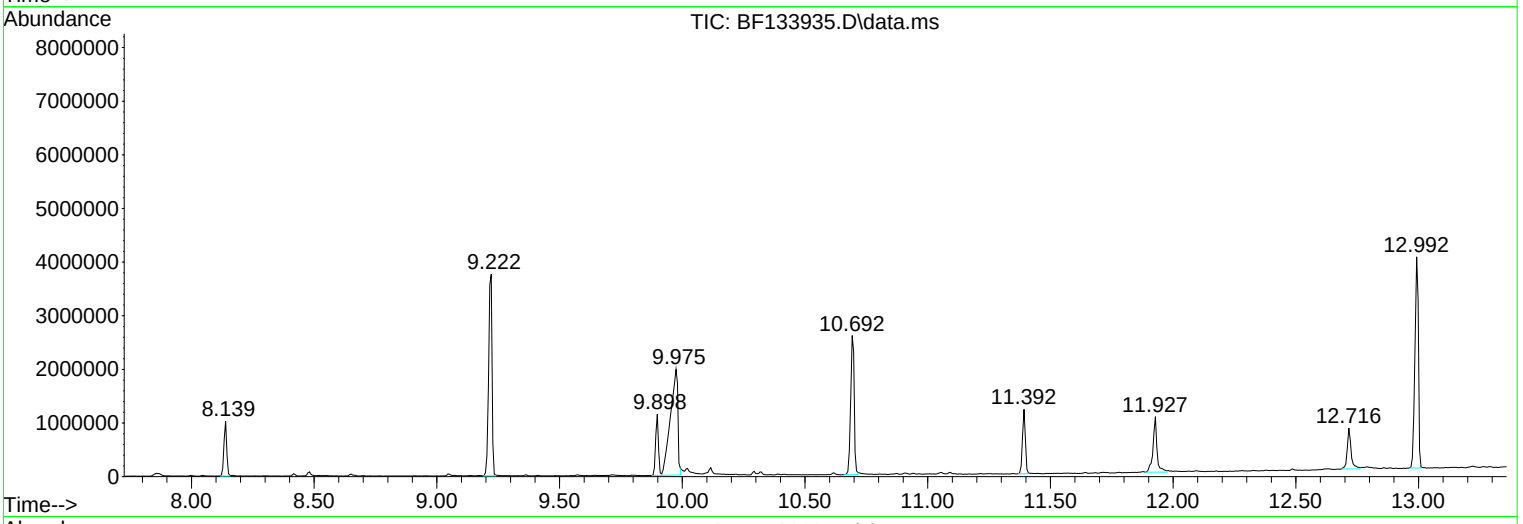
Misc :
ALS Vial : 6 Sample Multiplier: 1

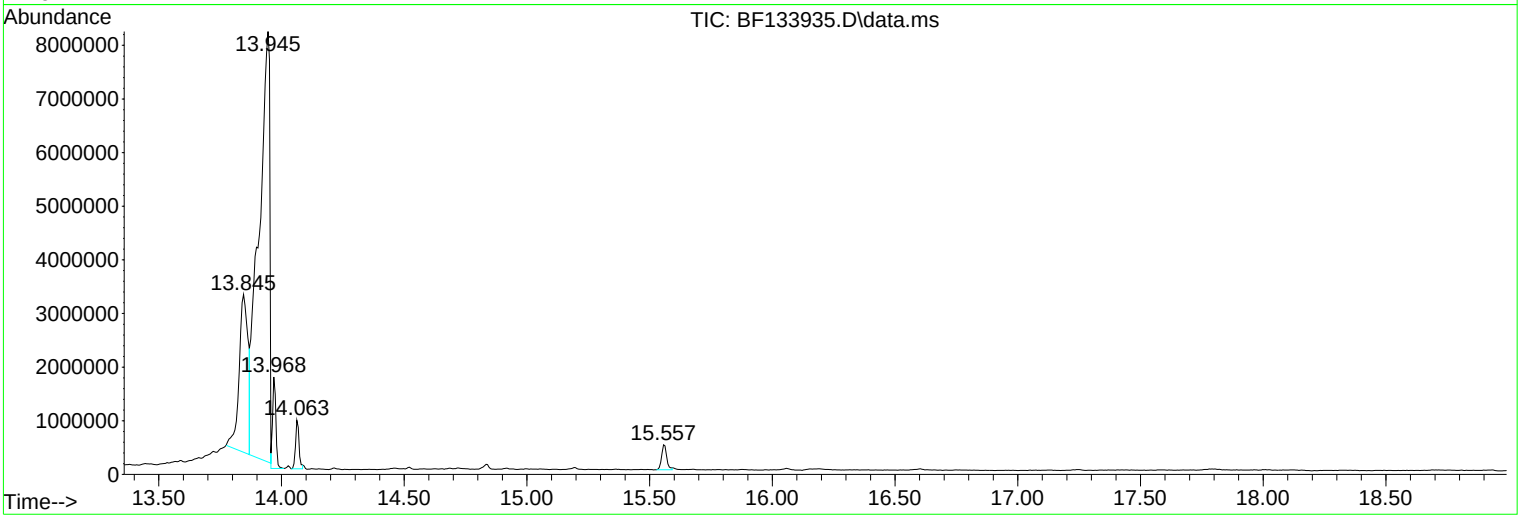
Instrument :
BNA_F
ClientSampleId :
TW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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

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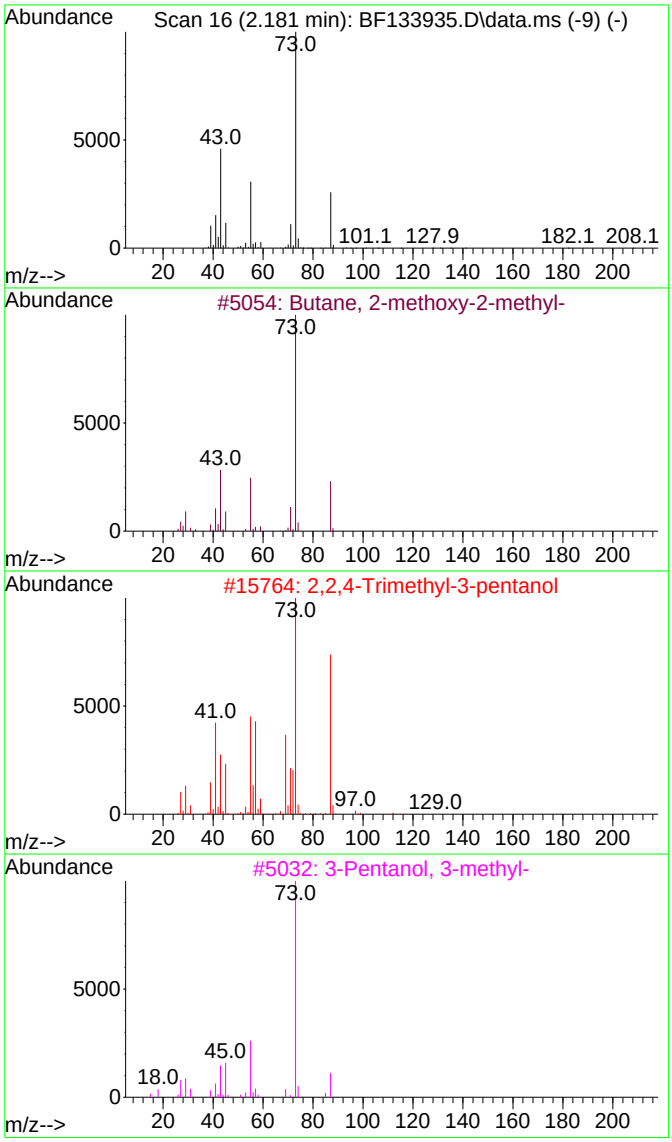
TIC Integration Parameters: LSCINT.P

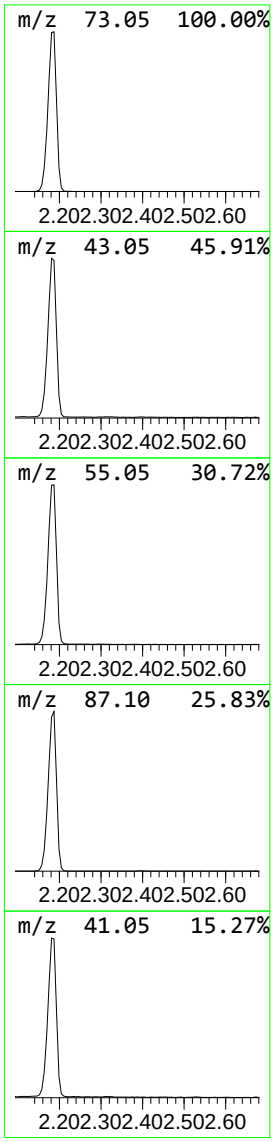
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	136.67 ng	4164890	1,4-Dichlorobenzene-d4	6.857

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	40
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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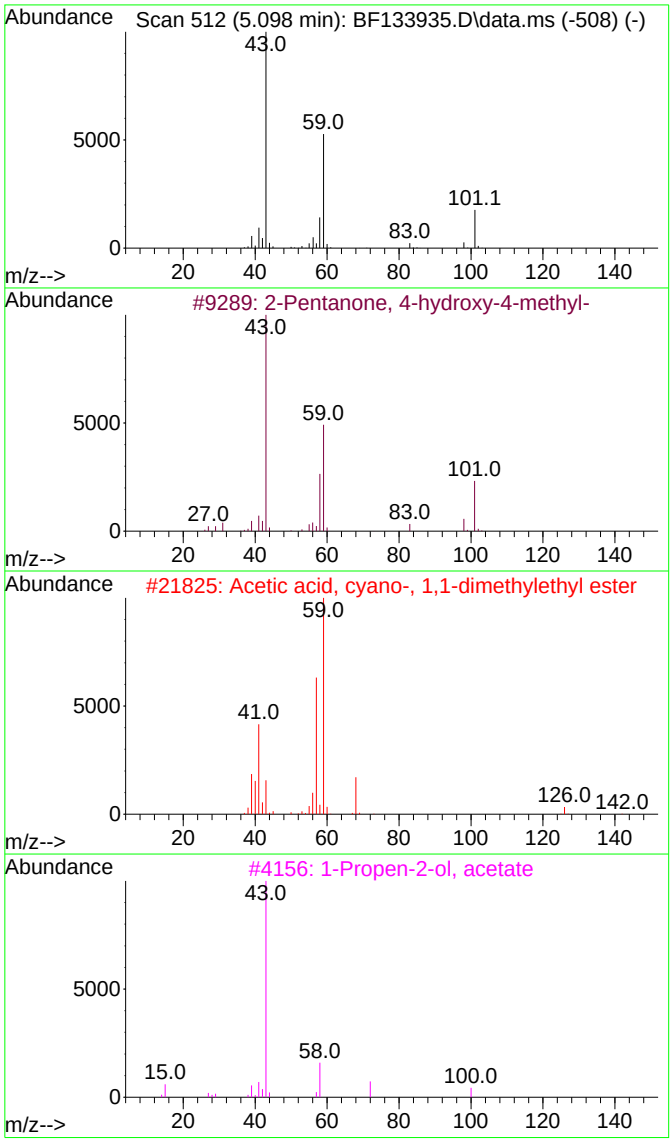
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

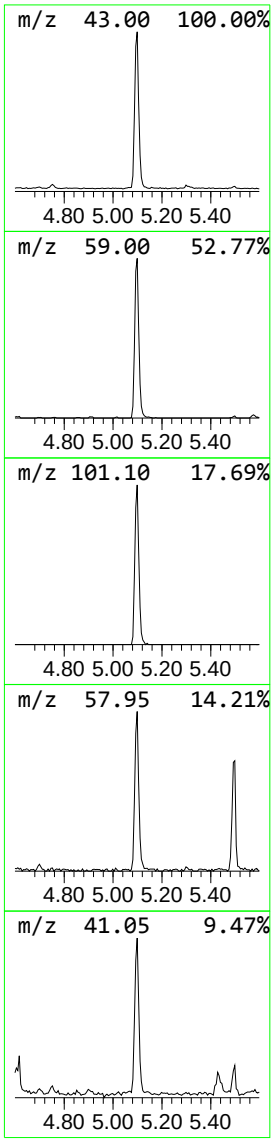
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	11.54 ng	351726	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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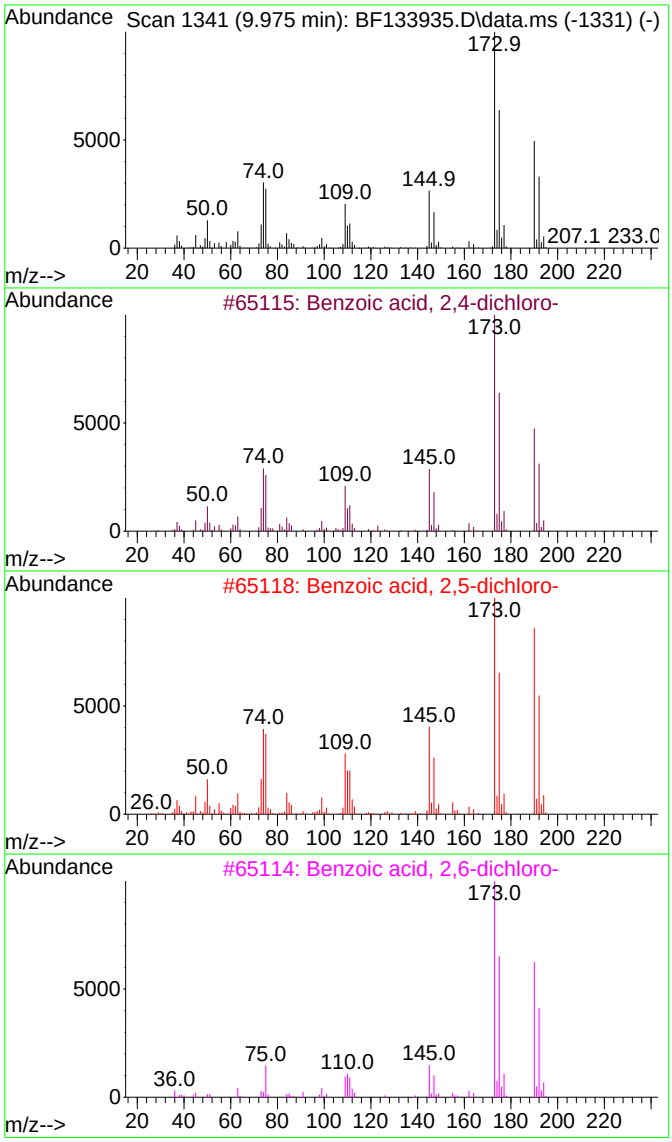
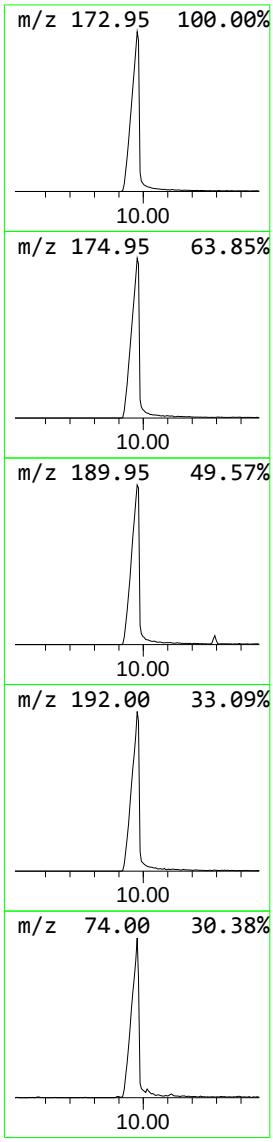
****
Peak Number 3 Benzoic acid, 2,4-dichloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.975	92.12 ng	4201380	Acenaphthene-d10	9.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4-dichloro-	190	C7H4Cl2O2	000050-84-0	99
2	Benzoic acid, 2,5-dichloro-	190	C7H4Cl2O2	000050-79-3	99
3	Benzoic acid, 2,6-dichloro-	190	C7H4Cl2O2	000050-30-6	98
4	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	97
5	Benzoic acid, 2,3-dichloro-	190	C7H4Cl2O2	000050-45-3	96





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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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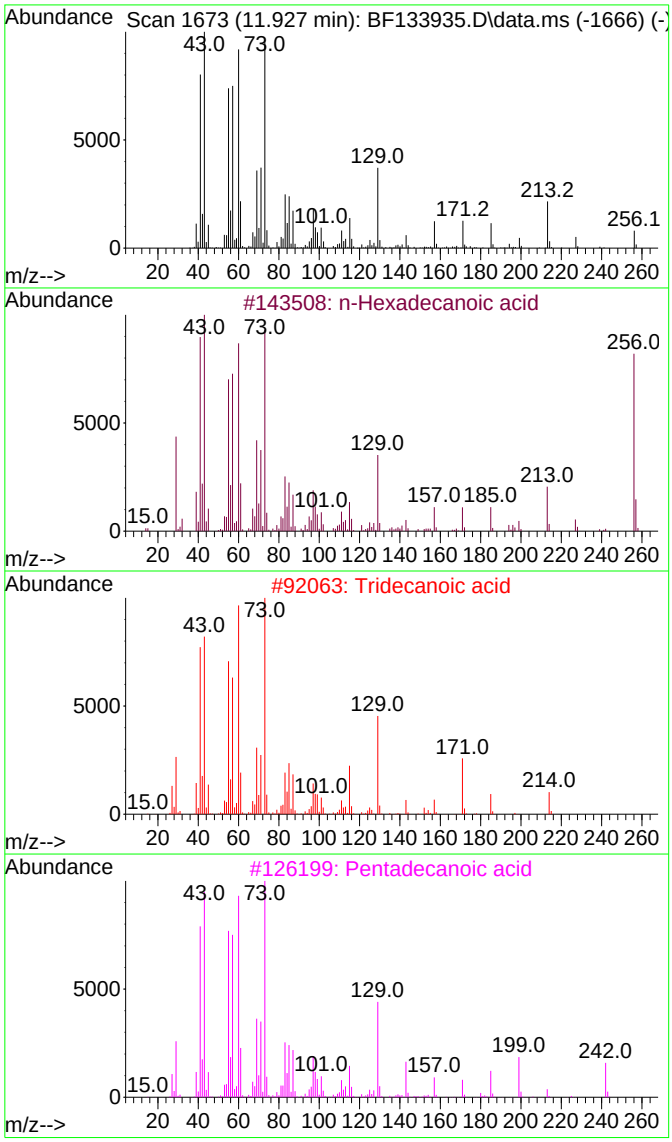
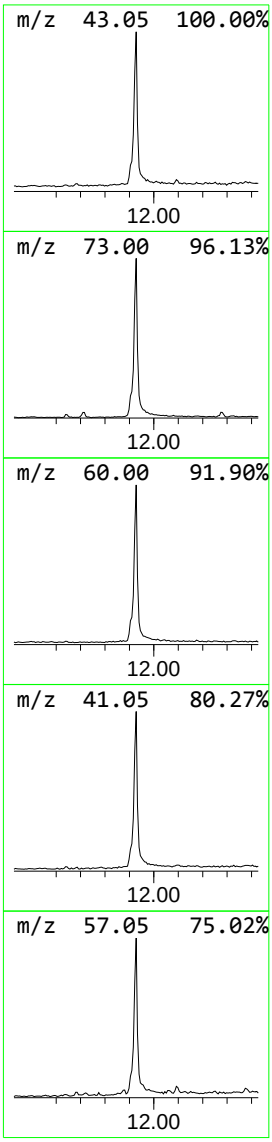
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	23.76 ng	1178140	Phenanthrene-d10	11.392

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	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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Instrument :
BNA_F
ClientSampleId :
TW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.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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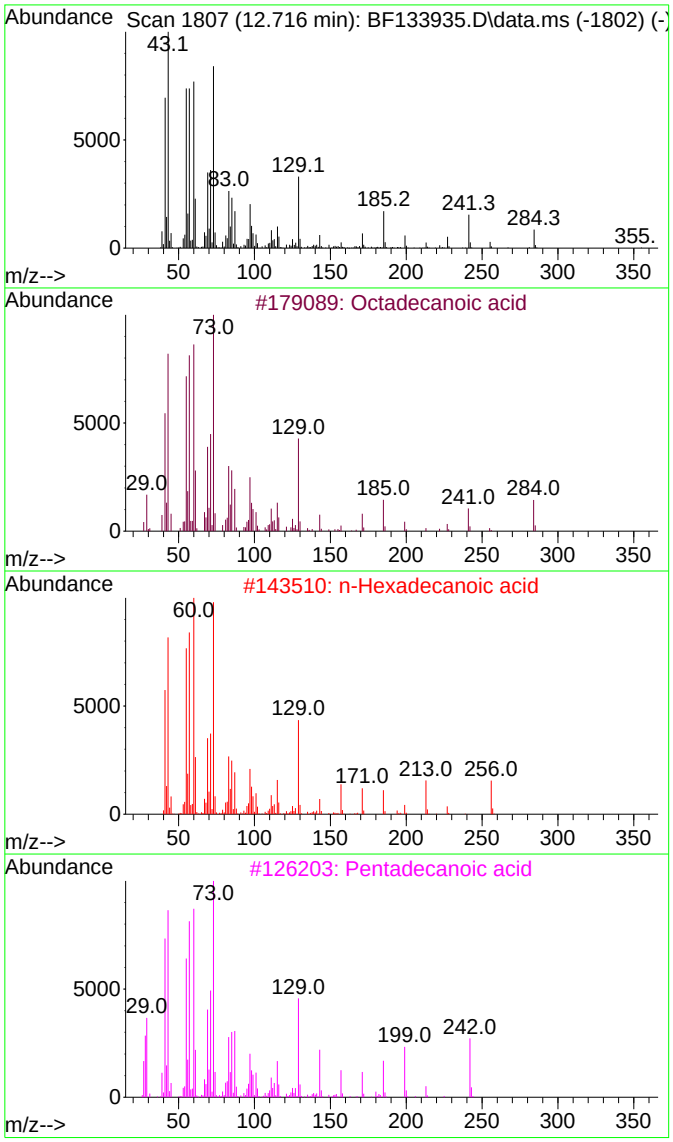
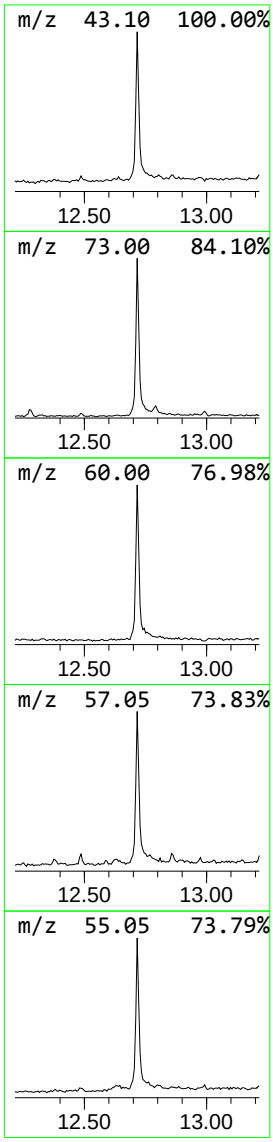
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	16.51 ng	818597	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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TIC Library : C:\Database\NIST20.L
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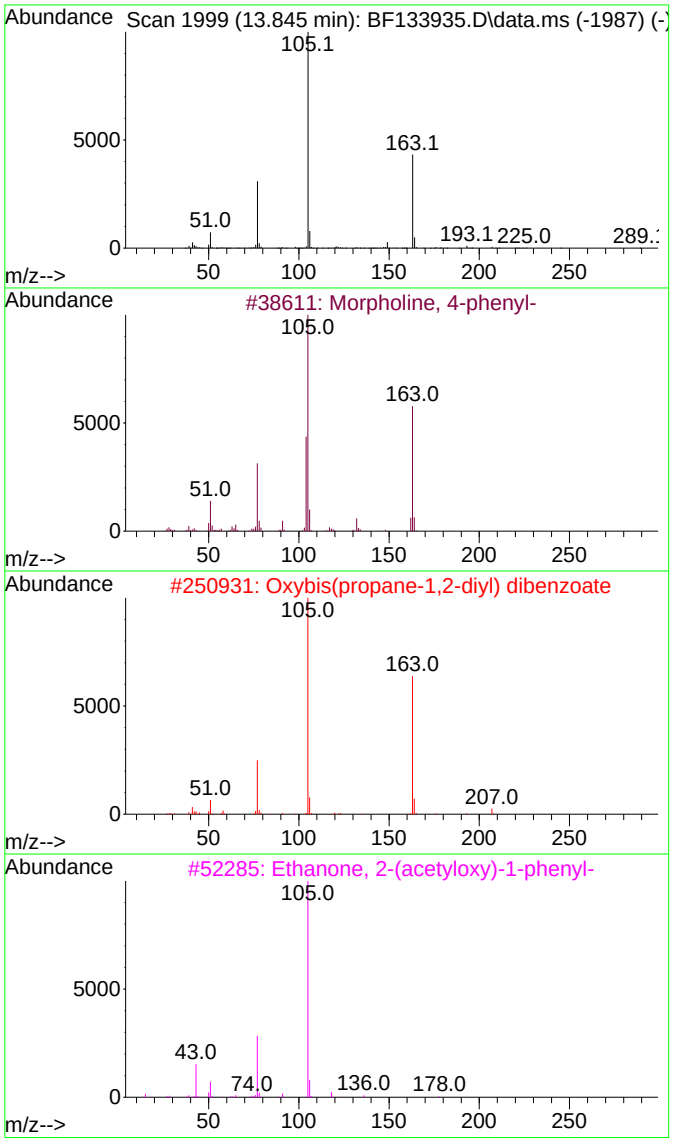
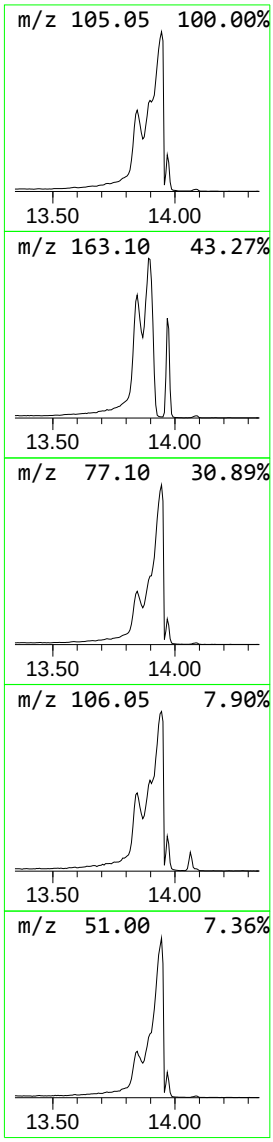
****

Peak Number 6 Morpholine, 4-phenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	167.35 ng	7522710	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
3	Ethanone, 2-(acetyloxy)-1-phenyl-	178	C10H10O3	002243-35-8	43
4	Phenylglyoxylic acid, isopropyl ...	192	C11H12O3	1000453-46-3	38
5	Benzoic acid, anhydride	226	C14H10O3	000093-97-0	38





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BNA_F
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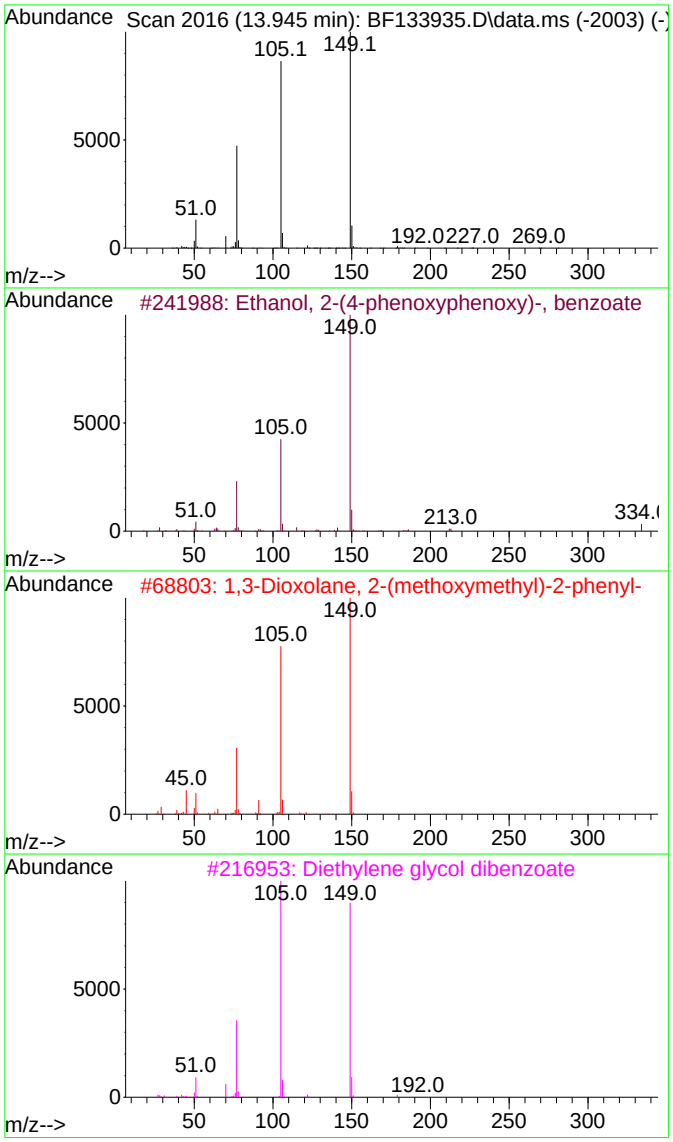
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

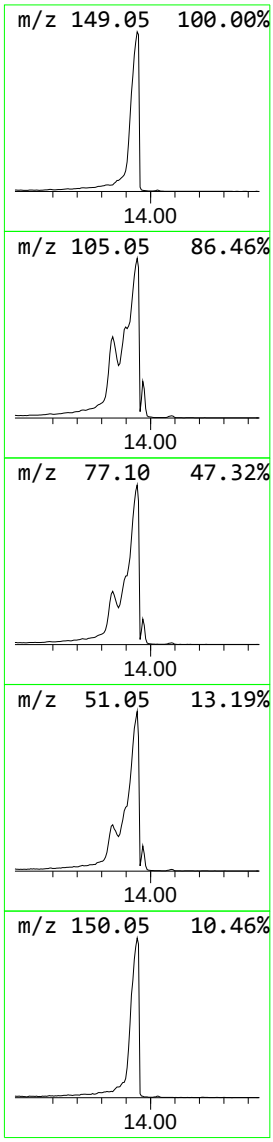
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethanol, 2-(4-phenoxyphenox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	549.38 ng	24695400	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	83
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
3	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
4	Benzamide, N,N-dimethyl-	149	C9H11NO	000611-74-5	64
5	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52





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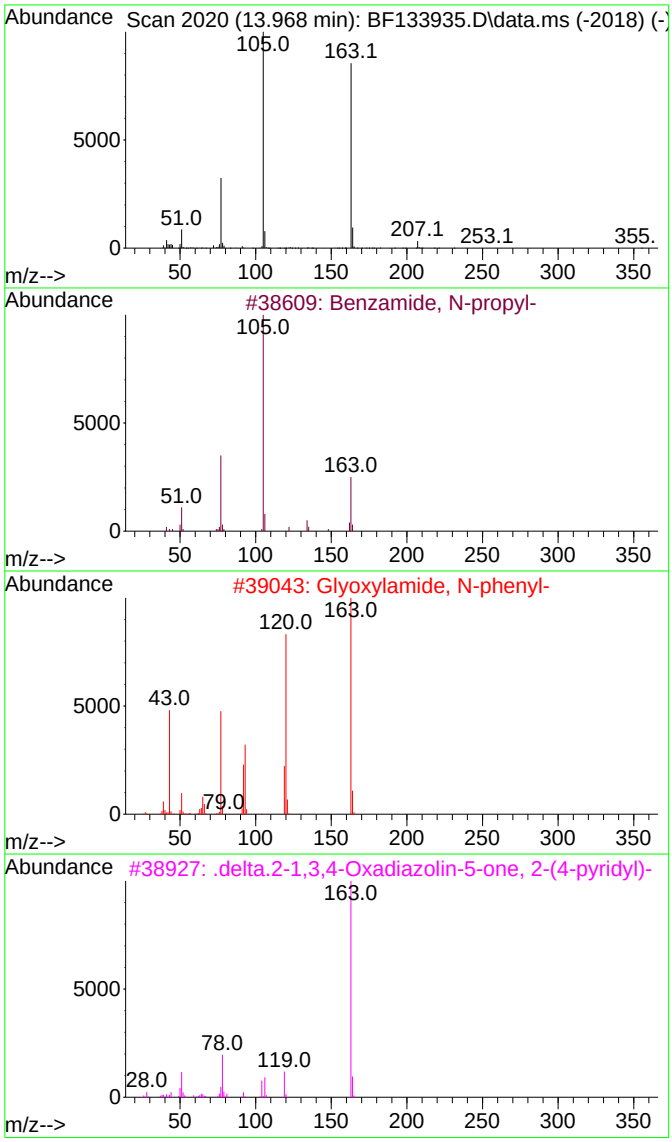
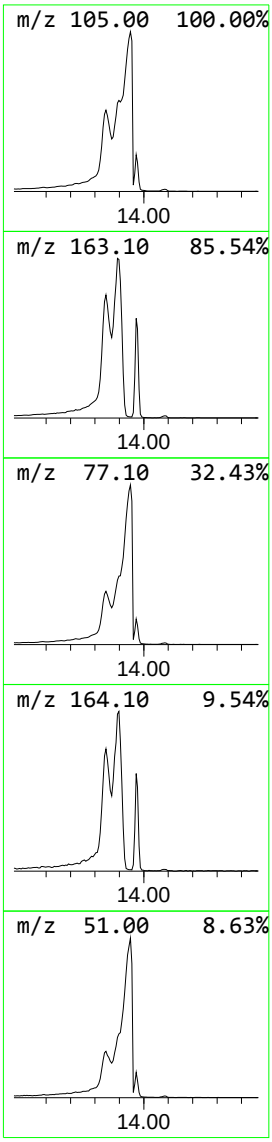
Peak Number 8 Benzamide, N-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	34.96 ng	1571300	Chrysene-d12	14.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	78
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	59
3	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	53
4	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	53
5	Phenylglyoxylic acid, pentyl ester	220	C13H16O3	1000453-46-0	22





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.181	136.7	ng	4164890	1	6.857	609473	20.0
2-Pentanone, 4-...	5.098	11.5	ng	351726	1	6.857	609473	20.0
Benzoic acid, 2...	9.975	92.1	ng	4201380	3	9.898	912118	20.0
n-Hexadecanoic ...	11.927	23.8	ng	1178140	4	11.392	991565	20.0
Octadecanoic acid	12.716	16.5	ng	818597	4	11.392	991565	20.0
Morpholine, 4-p...	13.845	167.3	ng	7522710	5	14.063	899033	20.0
Ethanol, 2-(4-p...	13.945	549.4	ng	24695400	5	14.063	899033	20.0
Benzamide, N-pr...	13.969	35.0	ng	1571300	5	14.063	899033	20.0