LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
Data File : BF136495.D
Acq On : 11 Dec 2023 17:42
Operator : CG\JU
Sample : 05551-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-110

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	11	rVB	2601050	3020740	70.65%	11.406%
2	5.034	496	501	509	rVB	516694	587958	13.75%	2.220%
3	5.440	565	570	573	rBV	2249545	1959824	45.83%	7.400%
4	6.434	734	739	742	rBV	1468172	1257509	29.41%	4.748%
5	6.792	796	800	804	rVB	971906	772304	18.06%	2.916%
6	7.357	890	896	899	rBV	2110505	2153941	50.37%	8.133%
7	8.069	1012	1017	1020	rBV	1247630	1050887	24.58%	3.968%
8	8.604	1105	1108	1116	rVB	55719	57628	1.35%	0.218%
9	9.151	1195	1201	1204	rBV	4708755	4275942	100.00%	16.146%
10	9.792	1307	1310	1312	rBV	108279	92077	2.15%	0.348%
11	9.828	1312	1316	1319	rVB	1512641	1184615	27.70%	4.473%
12	10.210	1374	1381	1385	rBV	544802	441371	10.32%	1.667%
13	10.622	1446	1451	1454	rBV	2680110	2506169	58.61%	9.463%
14	11.322	1566	1570	1573	rBV	1302405	1186283	27.74%	4.479%
15	11.457	1589	1593	1596	rVB	248418	191372	4.48%	0.723%
16	11.857	1657	1661	1672	rVB2	260070	271298	6.34%	1.024%
17	12.645	1791	1795	1802	rBV	176978	184000	4.30%	0.695%
18	12.916	1836	1841	1845	rBV	3670383	3713452	86.85%	14.022%
19	13.880	2001	2005	2016	rBV8	35617	95615	2.24%	0.361%
20	13.968	2016	2020	2024	rVV	809378	703153	16.44%	2.655%
21	14.451	2098	2102	2105	rBV	46982	50701	1.19%	0.191%
22	15.451	2266	2272	2277	rBV	559168	726485	16.99%	2.743%

Sum of corrected areas: 26483324

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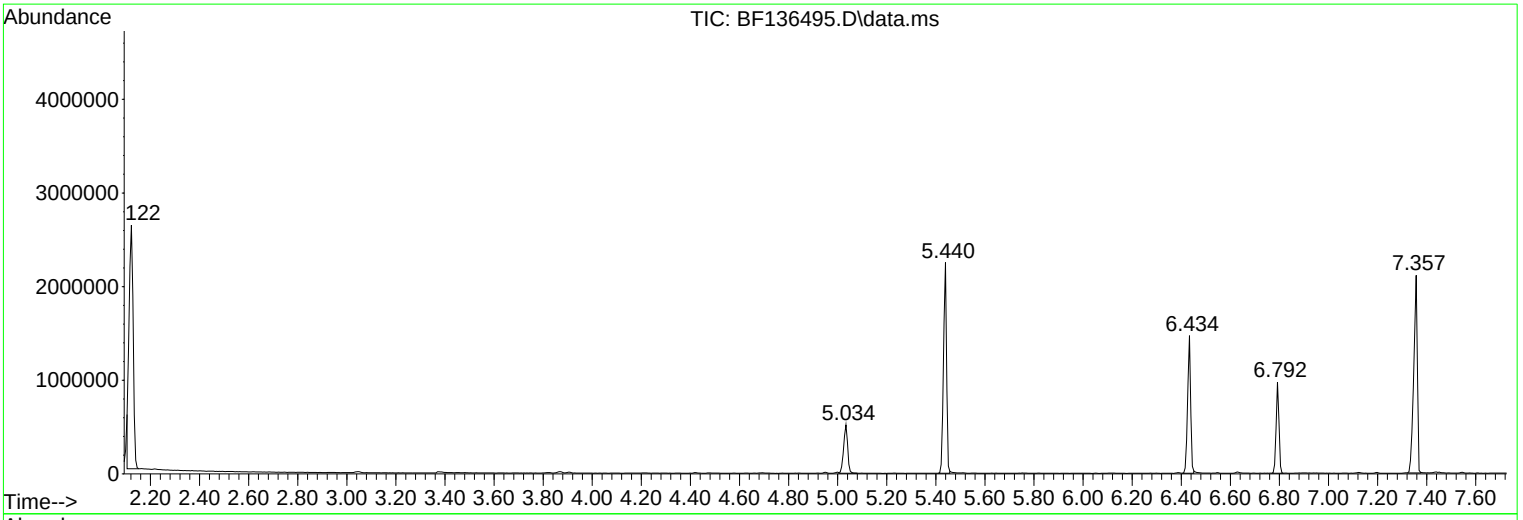
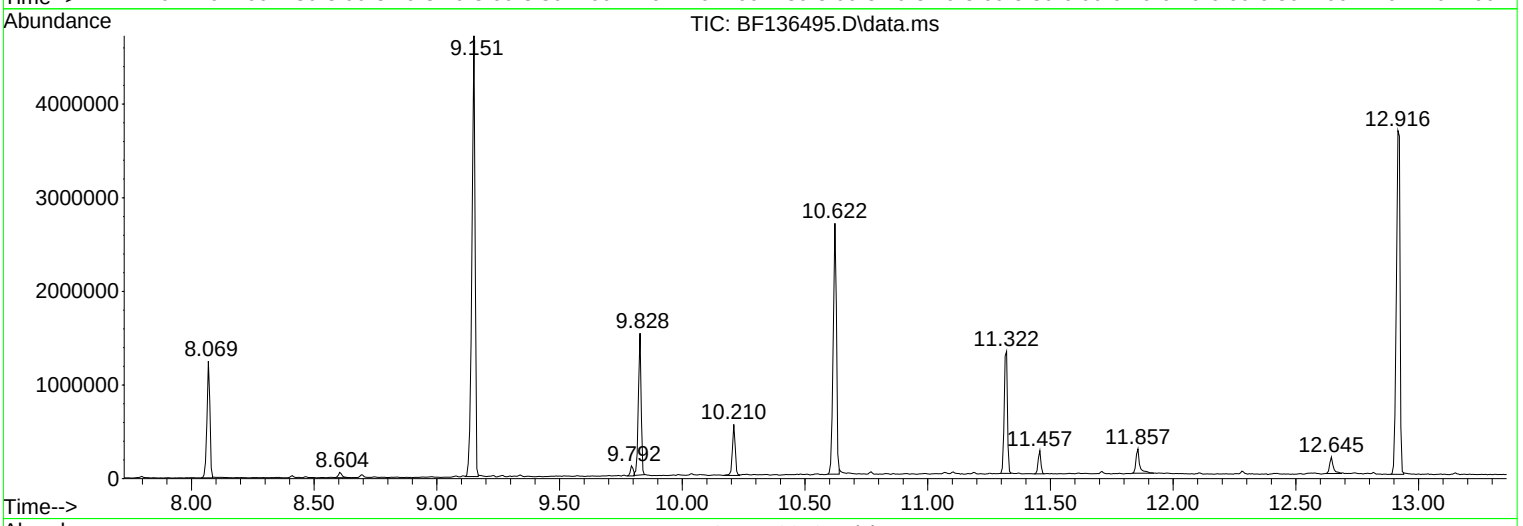
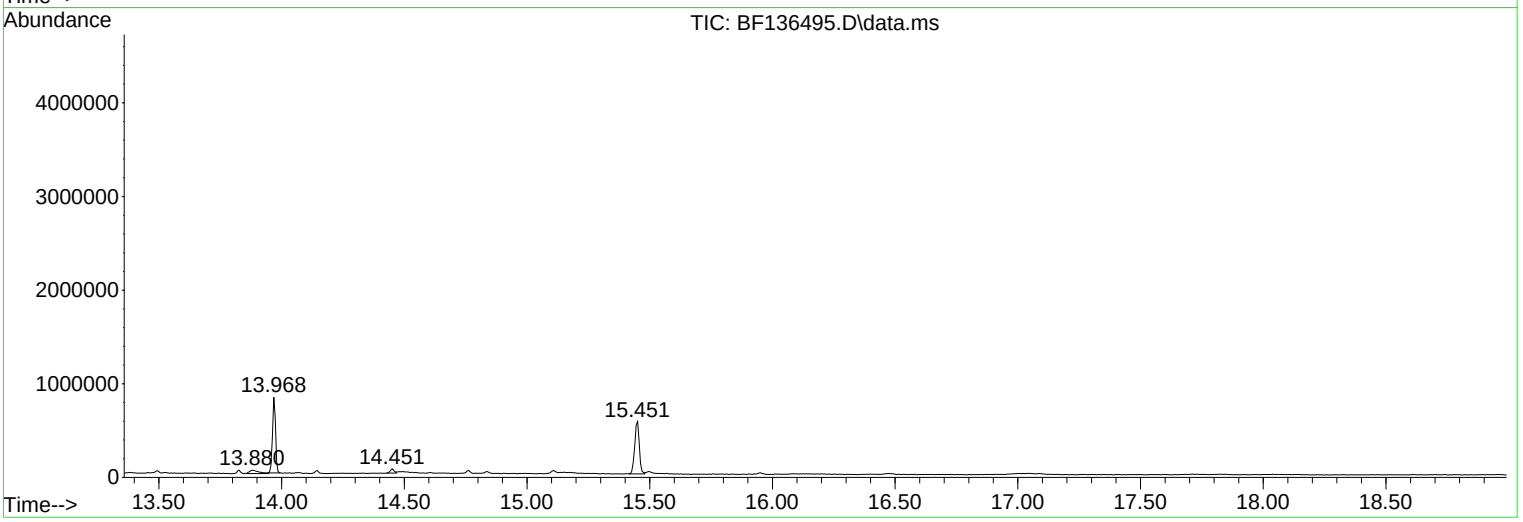
ClientSampleId :
MW-110

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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

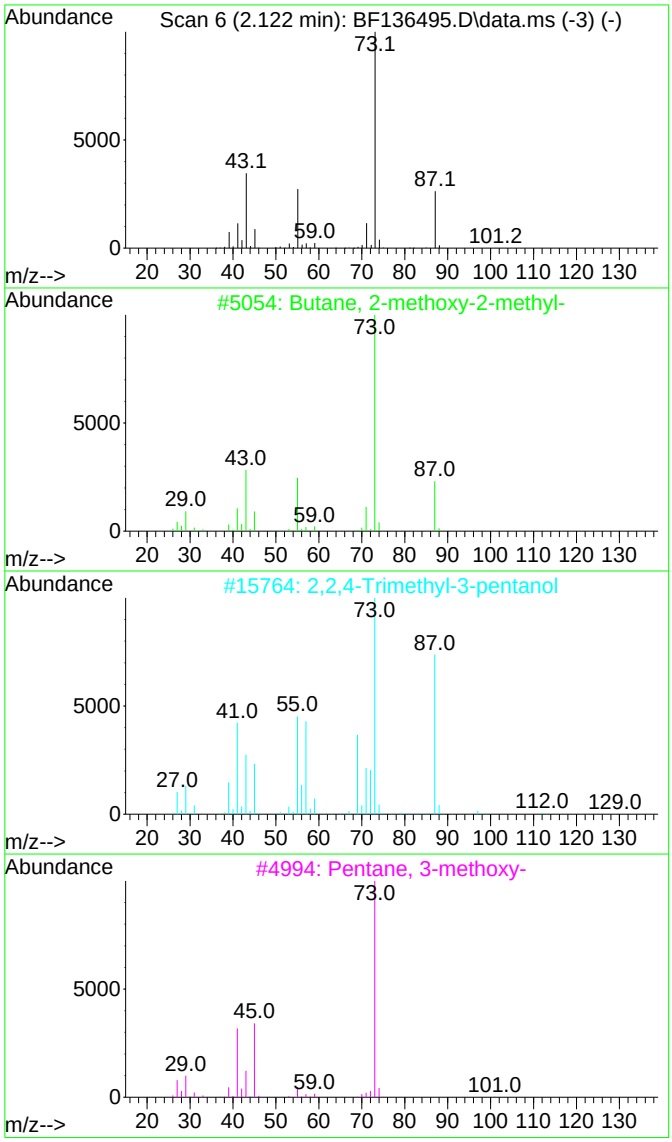
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

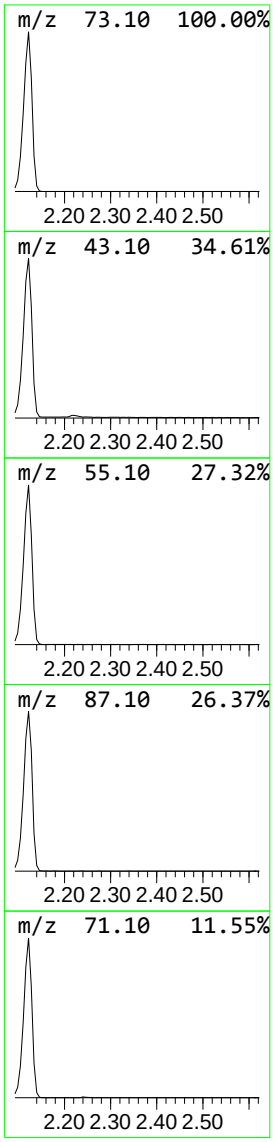
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	78.23 ng	3020740	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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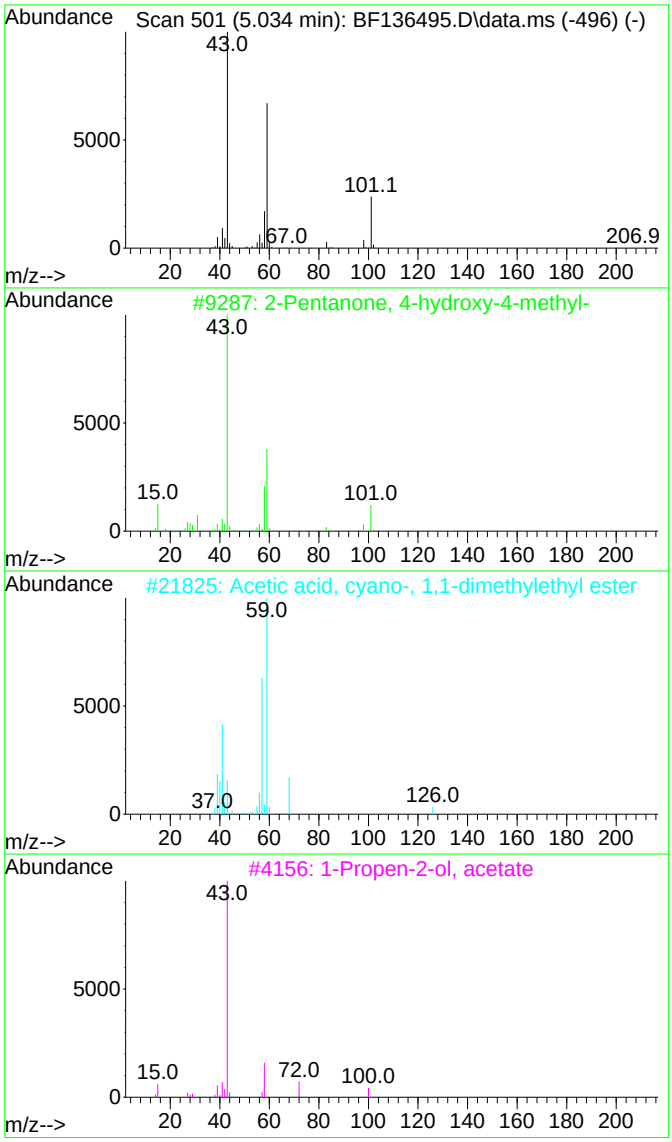
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

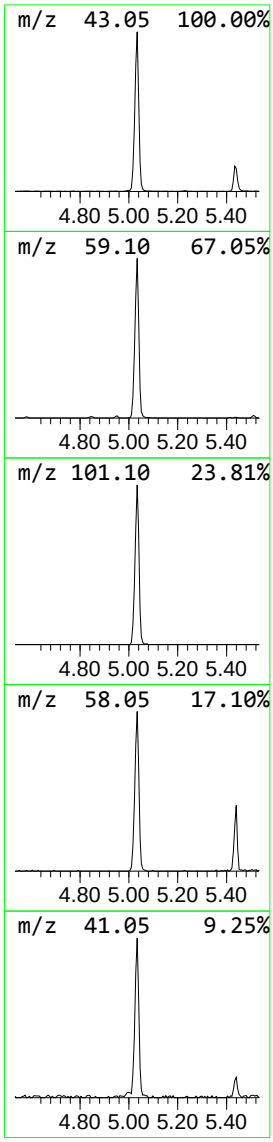
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	15.23 ng	587958	1,4-Dichlorobenzene-d4	6.792

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Sample : 05551-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-110

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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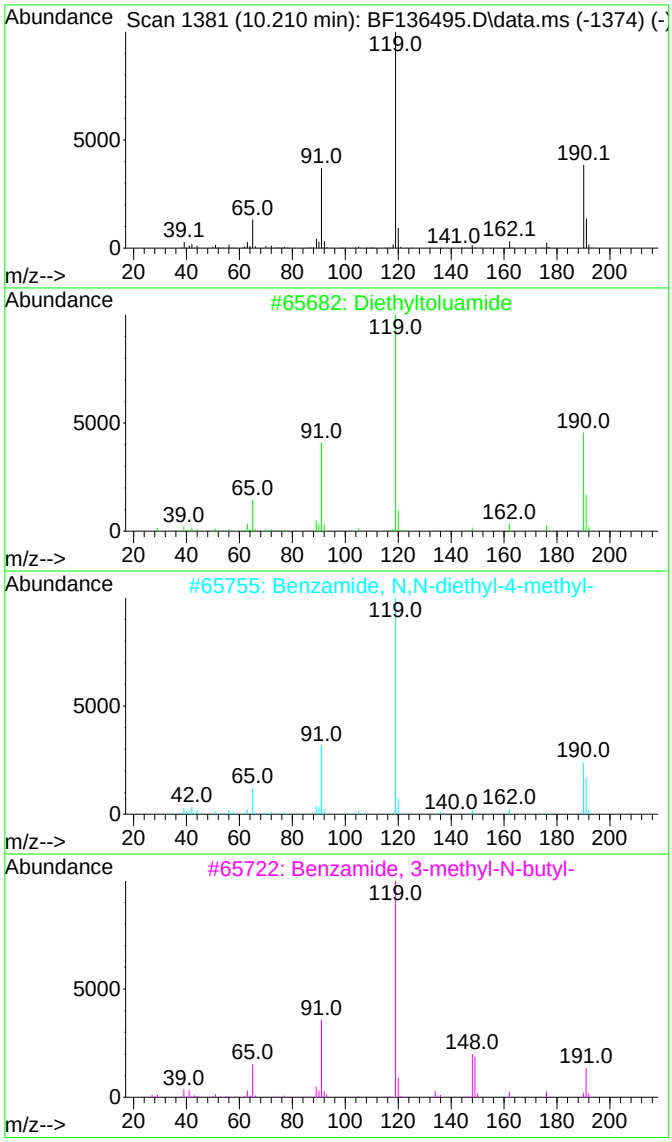
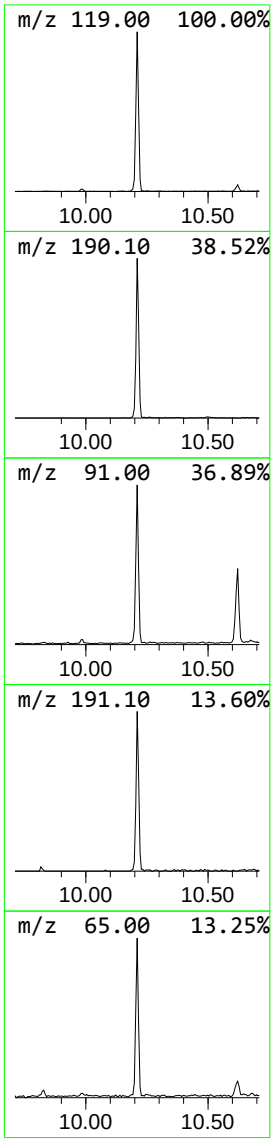
Peak Number 3 Diethyltoluamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.210	7.45 ng	441371	Acenaphthene-d10	9.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	93
3	Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76
4	Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	76
5	Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	76





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Instrument :
BNA_F
ClientSampleId :
MW-110

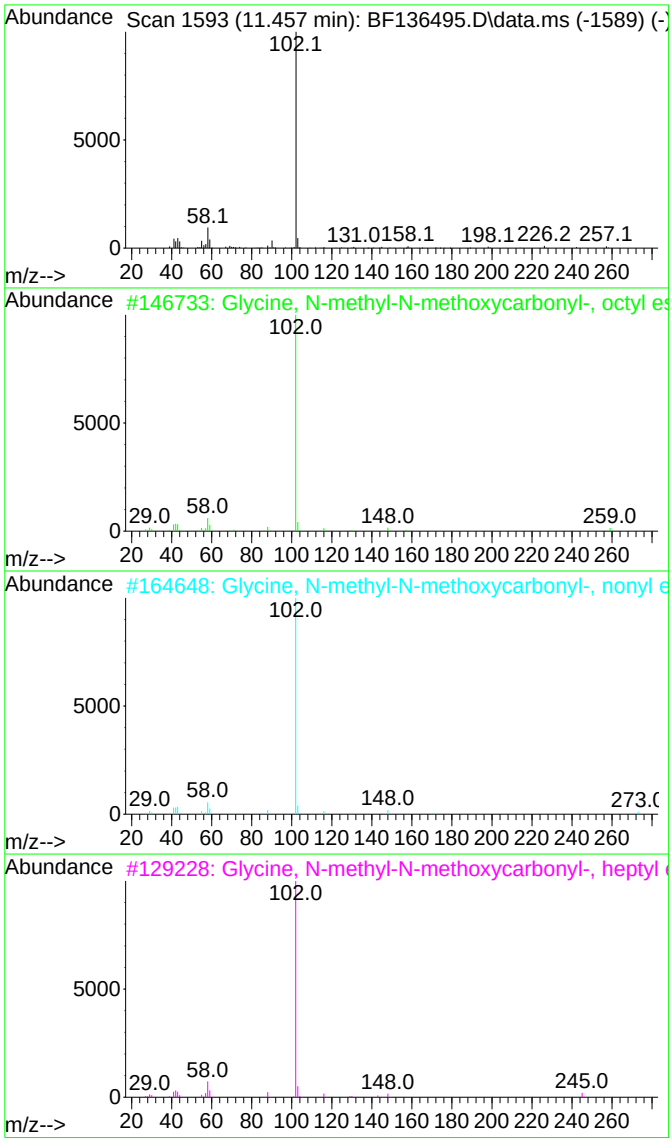
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

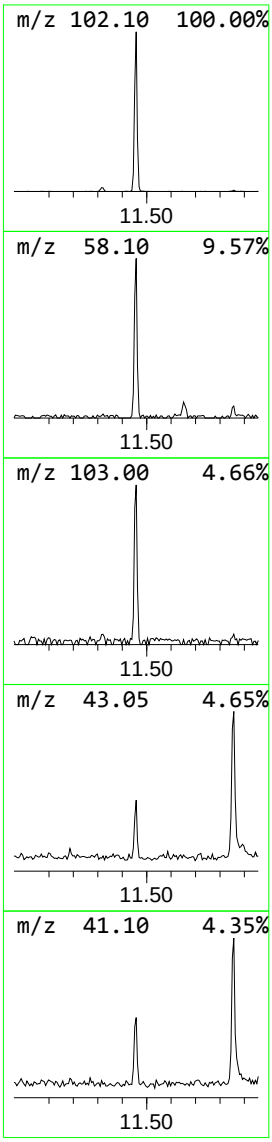
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Glycine, N-methyl-N-methoxy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.457	3.23 ng	191372	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycine, N-methyl-N-methoxycarbo...	259	C13H25NO4	1000320-60-9	72
2	Glycine, N-methyl-N-methoxycarbo...	273	C14H27NO4	1000320-61-0	72
3	Glycine, N-methyl-N-methoxycarbo...	245	C12H23NO4	1000320-60-8	72
4	Glycine, N-methyl-N-methoxycarbo...	203	C9H17NO4	1000320-60-3	72
5	l-Alanine, N-methoxycarbonyl-, t...	329	C18H35NO4	1010313-38-1	64





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TIC Integration Parameters: LSCINT.P

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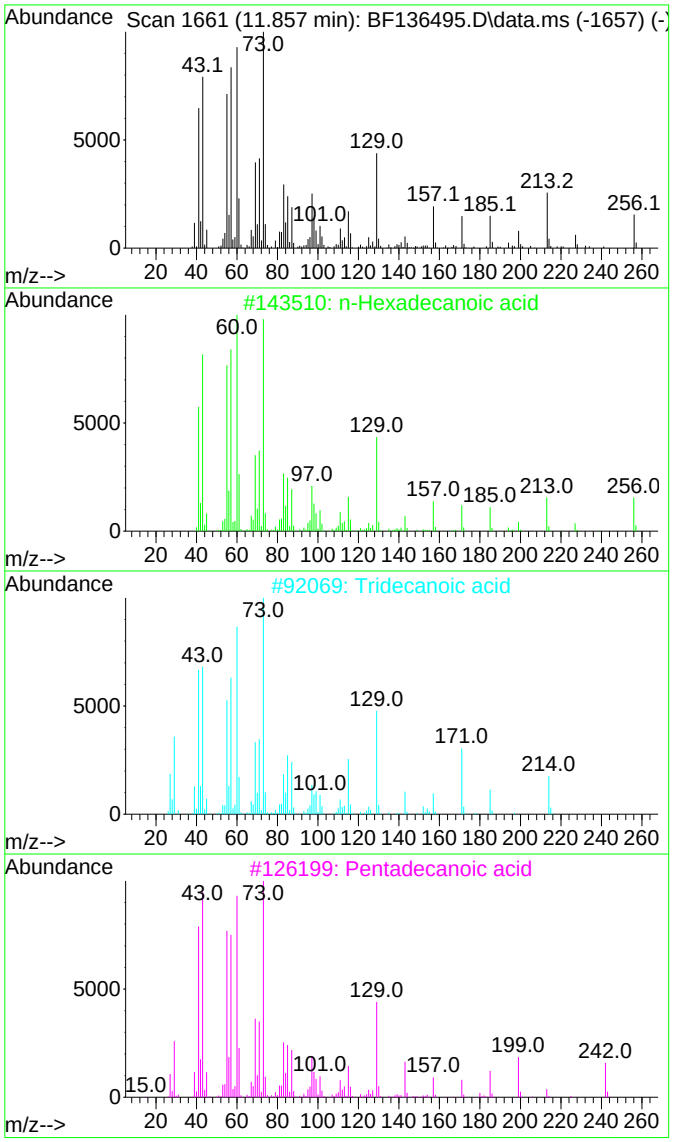
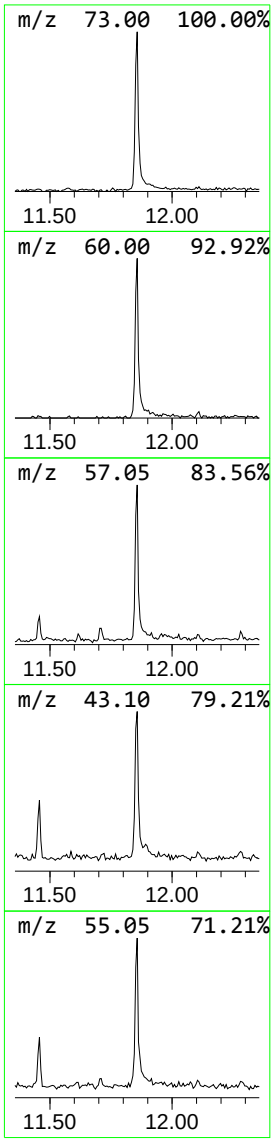
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.57 ng	271298	Phenanthrene-d10	11.322

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





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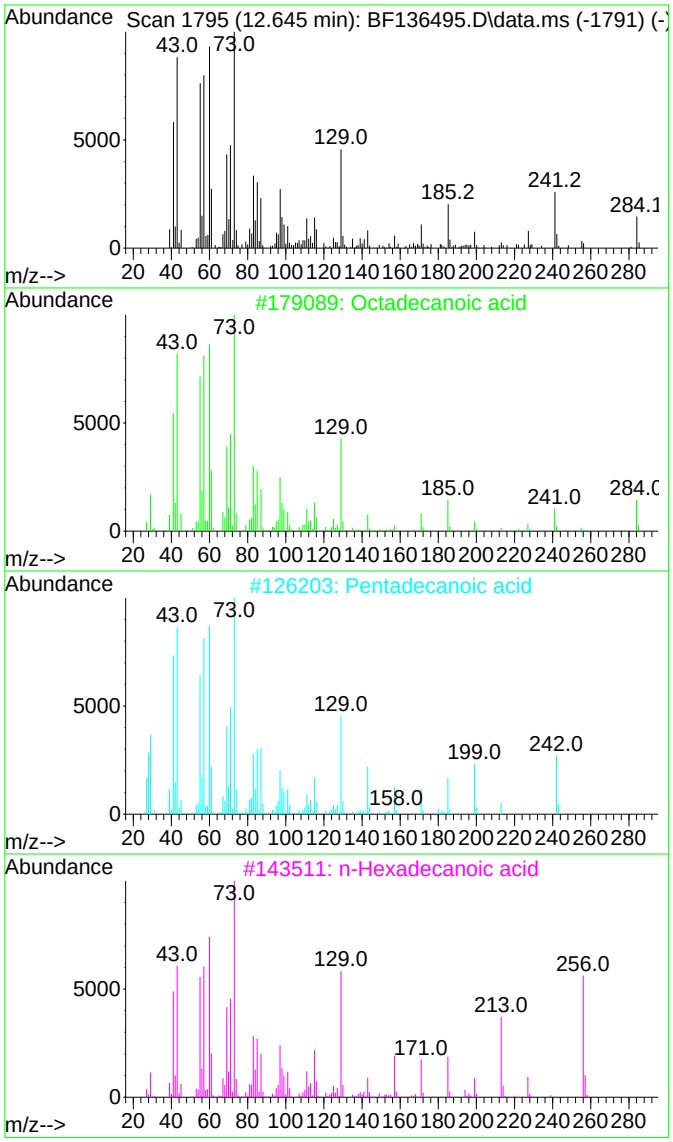
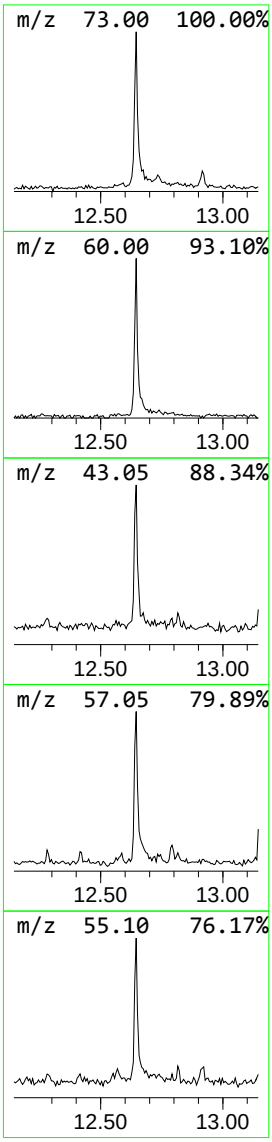
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	3.10 ng	184000	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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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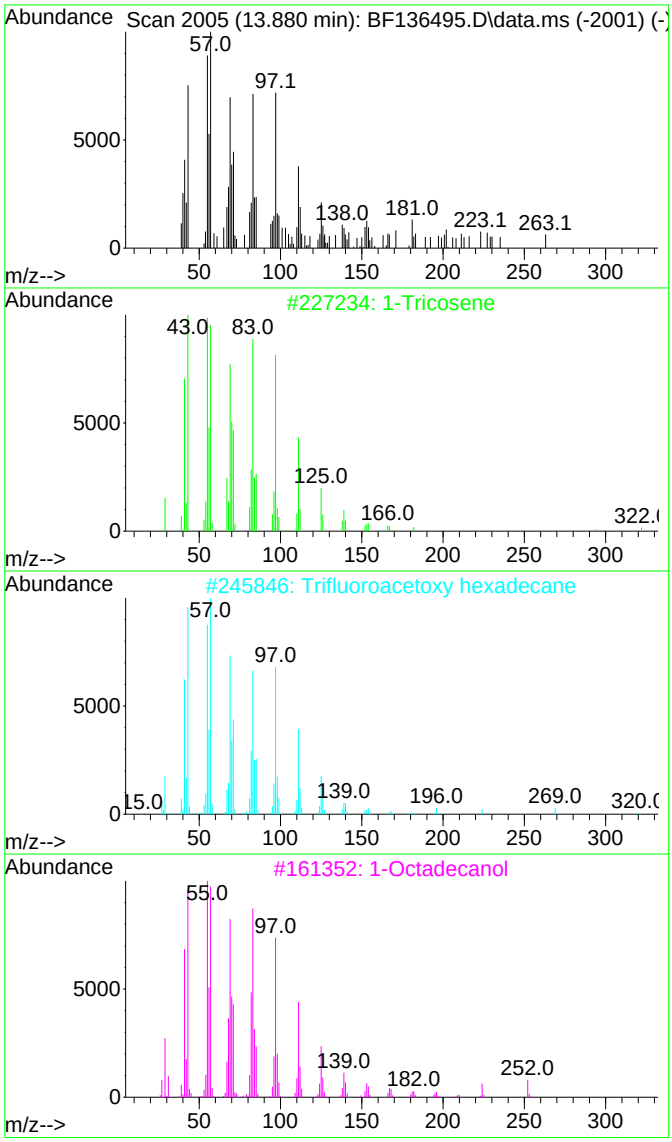
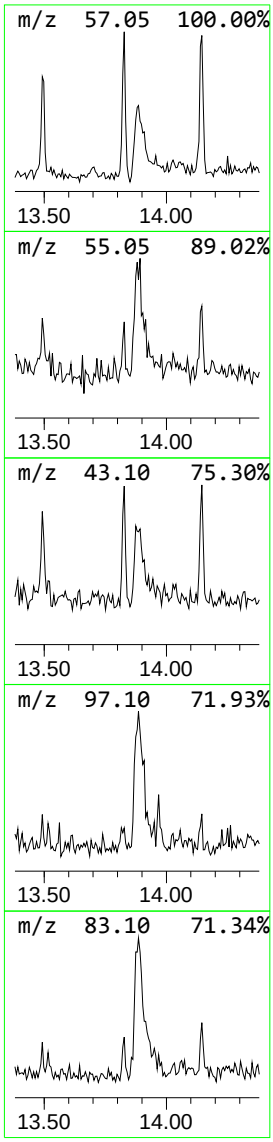
Peak Number 7 1-Tricosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.72 ng	95615	Chrysene-d12	13.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	1-Octadecanol	270	C18H38O	000112-92-5	94
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93





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...	2.122	78.2	ng	3020740	1	6.792	772304	20.0
2-Pentanone, 4-...	5.034	15.2	ng	587958	1	6.792	772304	20.0
Diethyltoluamide	10.210	7.5	ng	441371	3	9.828	1184620	20.0
Glycine, N-meth...	11.457	3.2	ng	191372	4	11.322	1186280	20.0
n-Hexadecanoic ...	11.857	4.6	ng	271298	4	11.322	1186280	20.0
Octadecanoic acid	12.645	3.1	ng	184000	4	11.322	1186280	20.0
1-Tricosene	13.880	2.7	ng	95615	5	13.968	703153	20.0