LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100423\
Data File : BF135582.D
Acq On : 04 Oct 2023 21:46
Operator : CG\JU
Sample : 04687-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HR-3-092923

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135582.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.722	104	108	116	rVB	304871	432138	9.35%	1.268%
2	3.487	232	238	250	rBV	253375	438638	9.49%	1.287%
3	3.981	317	322	329	rBV	51030	77164	1.67%	0.226%
4	4.363	382	387	401	rBV	1781349	2324867	50.28%	6.821%
5	4.557	417	420	426	rBV	90588	106522	2.30%	0.313%
6	4.616	426	430	447	rVB2	114982	236043	5.10%	0.693%
7	4.992	490	494	508	rBV	515343	723978	15.66%	2.124%
8	5.386	558	561	583	rBV	3969390	4284787	92.67%	12.572%
9	6.363	723	727	728	rBV	104729	87488	1.89%	0.257%
10	6.392	728	732	759	rVB	3672716	4010010	86.72%	11.766%
11	6.739	787	791	801	rBV	1110953	937536	20.28%	2.751%
12	7.304	883	887	890	rBV	2945981	2888533	62.47%	8.475%
13	8.016	1004	1008	1023	rVB	1320371	1226440	26.52%	3.598%
14	9.092	1186	1191	1194	rBV	4508008	4623845	100.00%	13.567%
15	9.769	1302	1306	1316	rBV	1408633	1301689	28.15%	3.819%
16	10.569	1437	1442	1458	rBV	2884485	3074142	66.48%	9.020%
17	11.263	1557	1560	1569	rBV	1678173	1421826	30.75%	4.172%
18	11.804	1648	1652	1663	rBV2	84365	169206	3.66%	0.496%
19	12.862	1827	1832	1835	rBV	4306156	4507285	97.48%	13.225%
20	13.921	2009	2012	2024	rVB	864889	824975	17.84%	2.421%
21	15.386	2257	2261	2273	rBV2	235635	385235	8.33%	1.130%

Sum of corrected areas: 34082347

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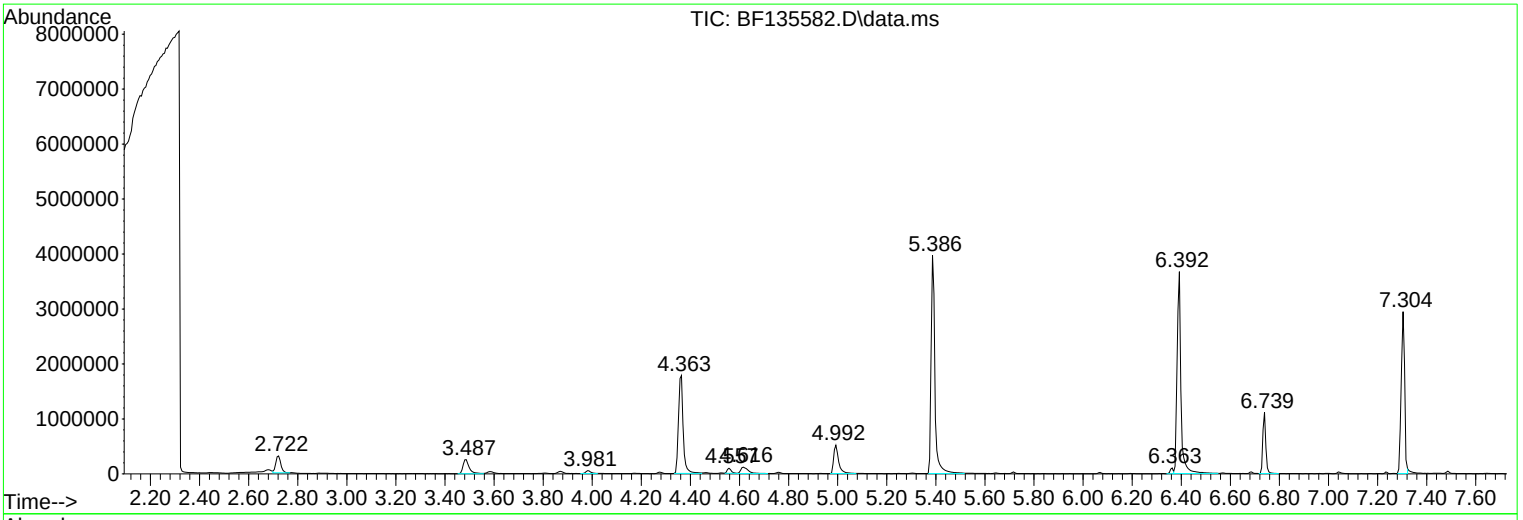
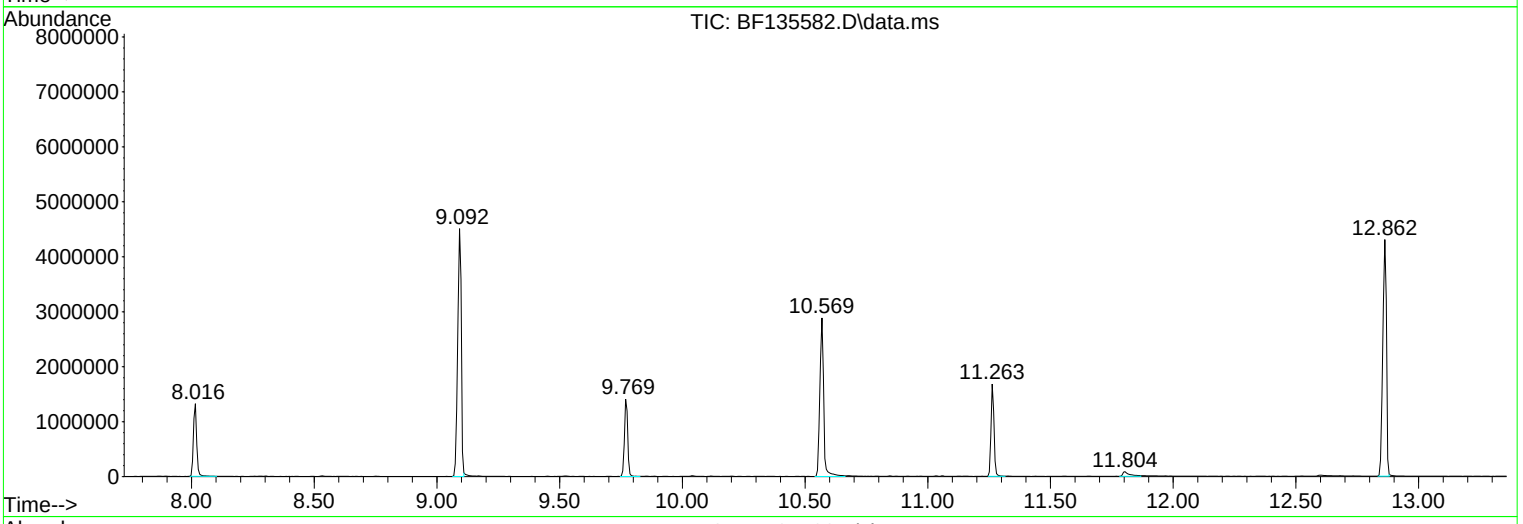
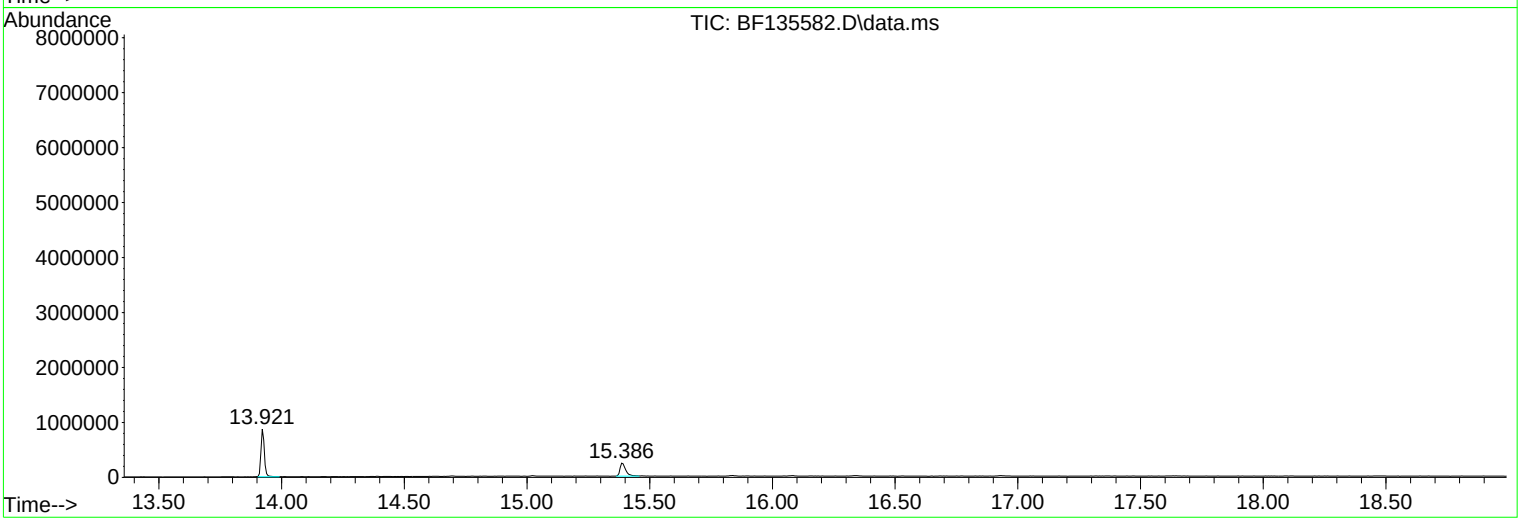
Instrument :
BNA_F
ClientSampleId :
HR-3-092923

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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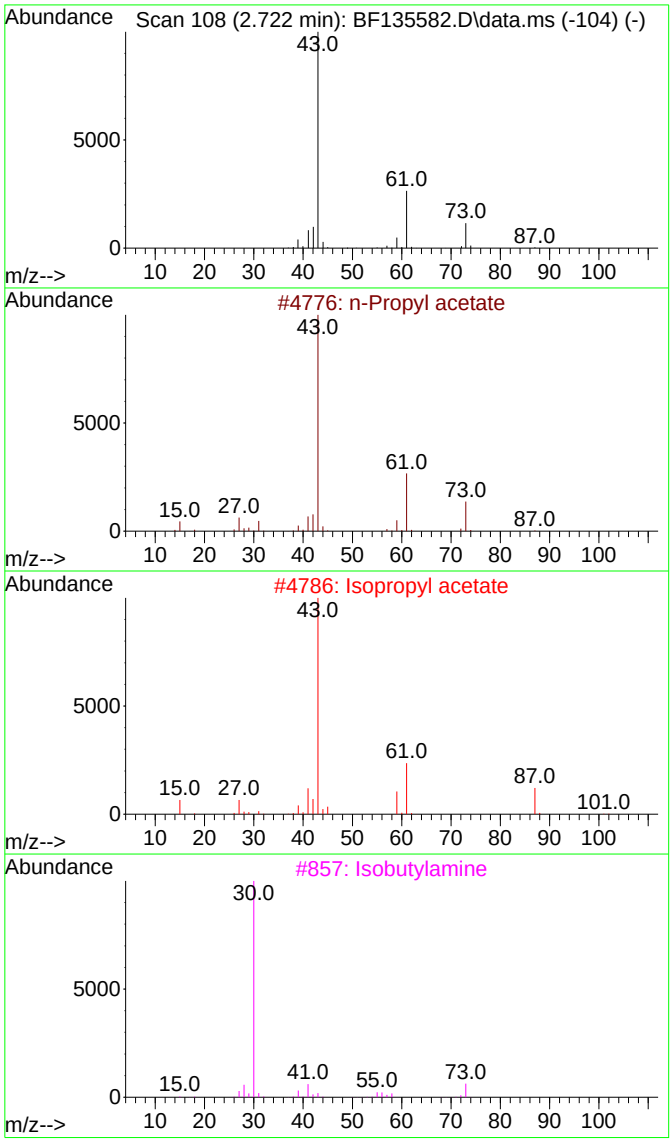
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

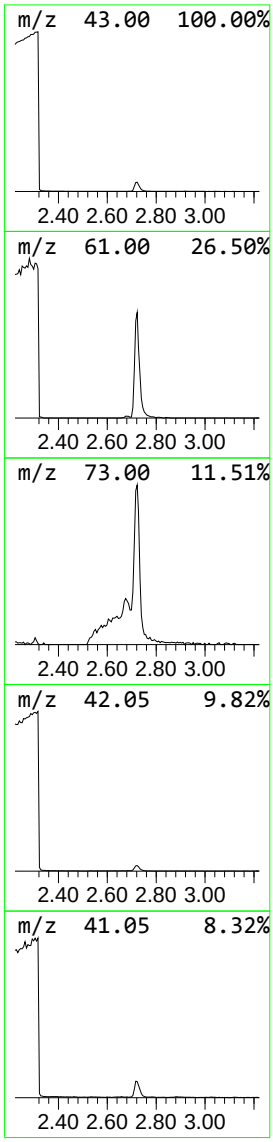
****

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.722	9.22 ng	432138	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Isopropyl acetate	102	C5H10O2	000108-21-4	9
3	Isobutylamine	73	C4H11N	000078-81-9	7
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

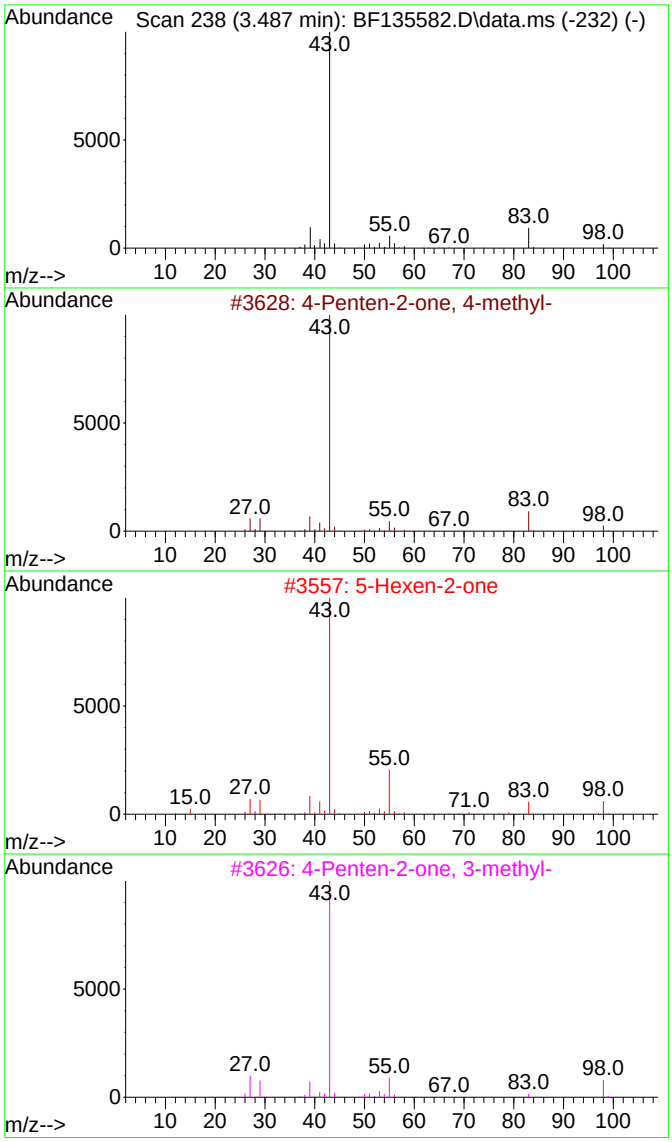
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

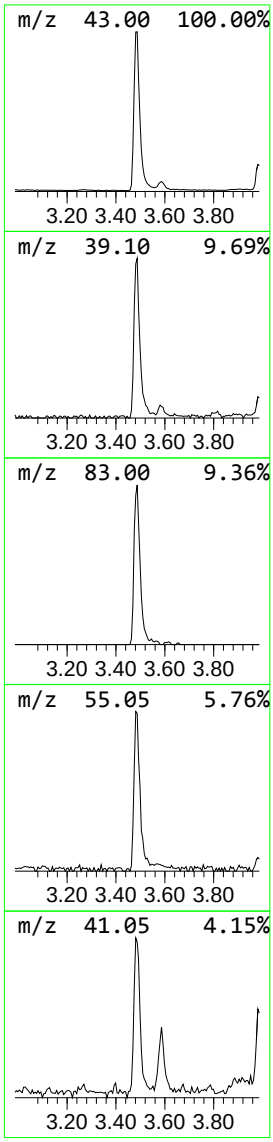
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.487	9.36 ng	438638	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	40
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9
4	4-Hexen-2-one	98	C6H10O	025659-22-7	9
5	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9





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Operator : CG\JU
Sample : 04687-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HR-3-092923

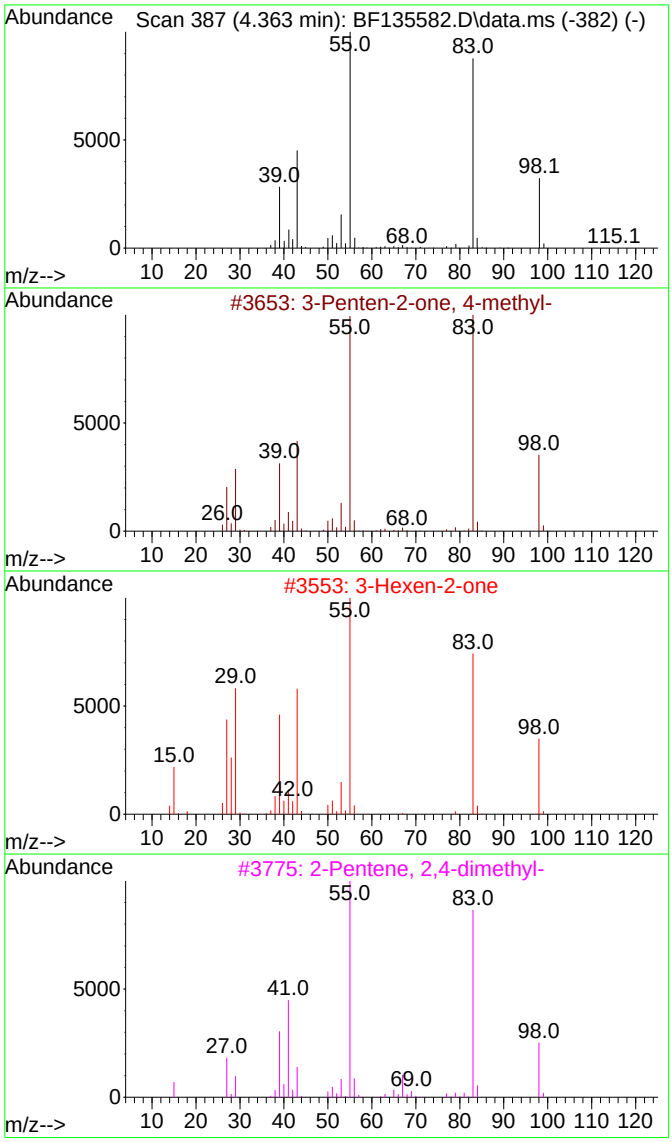
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

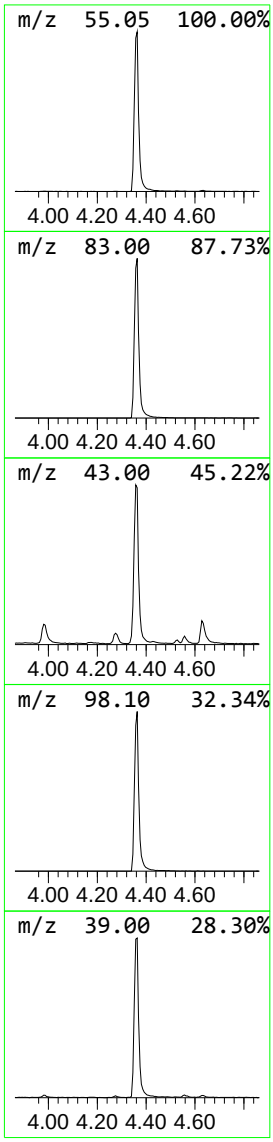
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.363	49.60 ng	2324870	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78





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Instrument :
BNA_F
ClientSampleId :
HR-3-092923

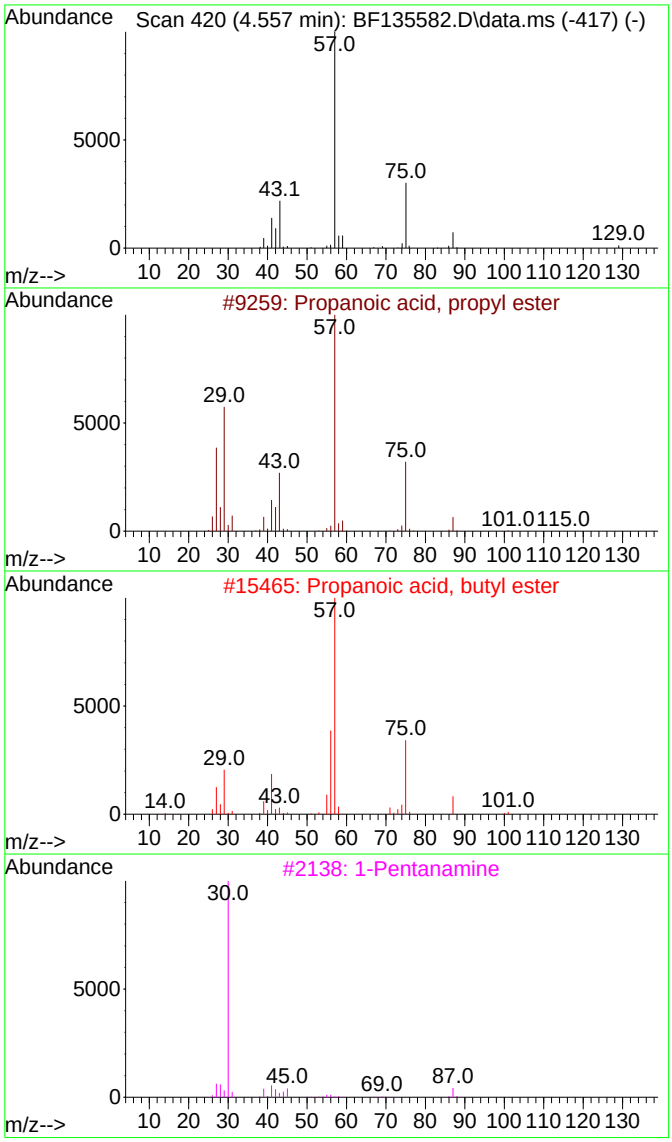
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

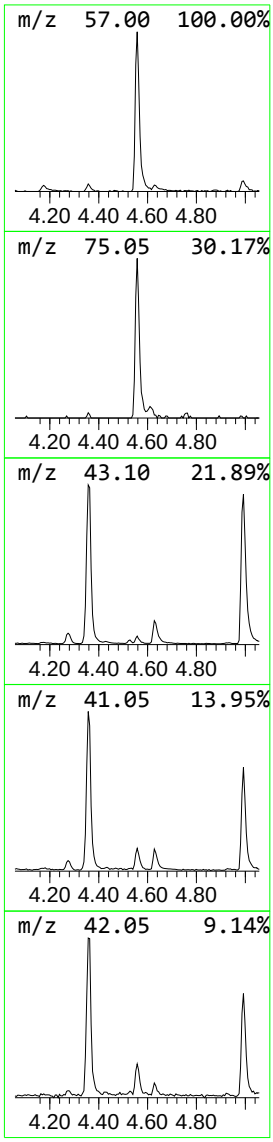
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	2.27 ng	106522	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36
3	1-Pentanamine	87	C5H13N	000110-58-7	9
4	Propionic acid, 4-hydroxy-3-hexy...	174	C9H18O3	1000151-16-9	9
5	O-tert-Butyl-L-threonine	175	C8H17NO3	004378-13-6	9





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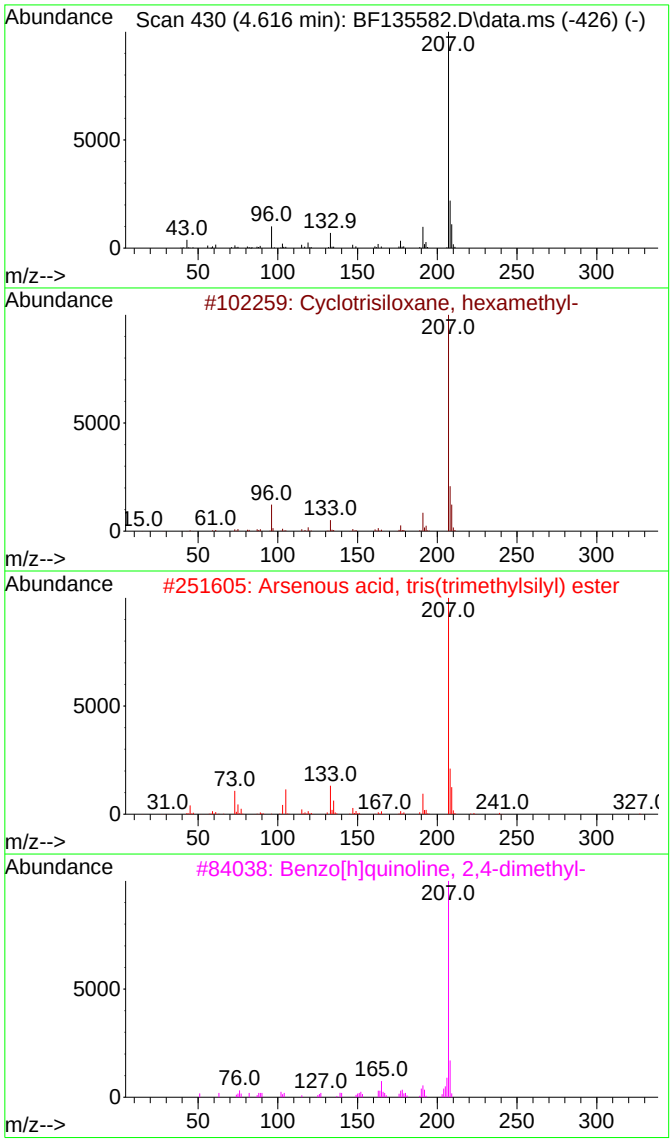
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

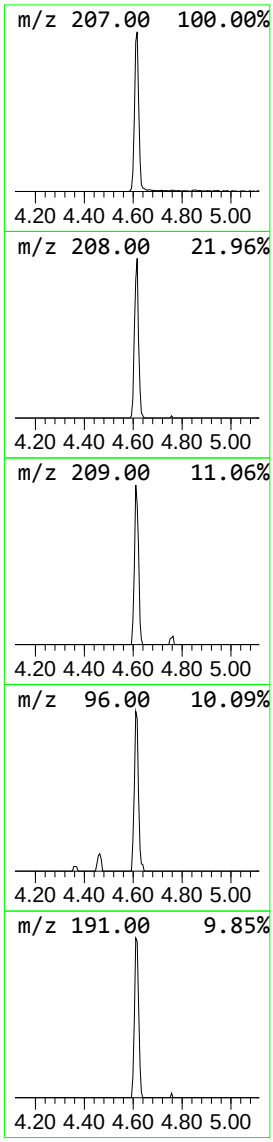
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclotrisiloxane, hexamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.616	5.04 ng	236043	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	72
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	39
5	4-tert-Octylphenol, TMS derivative	278	C17H30OSi	078721-87-6	39





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

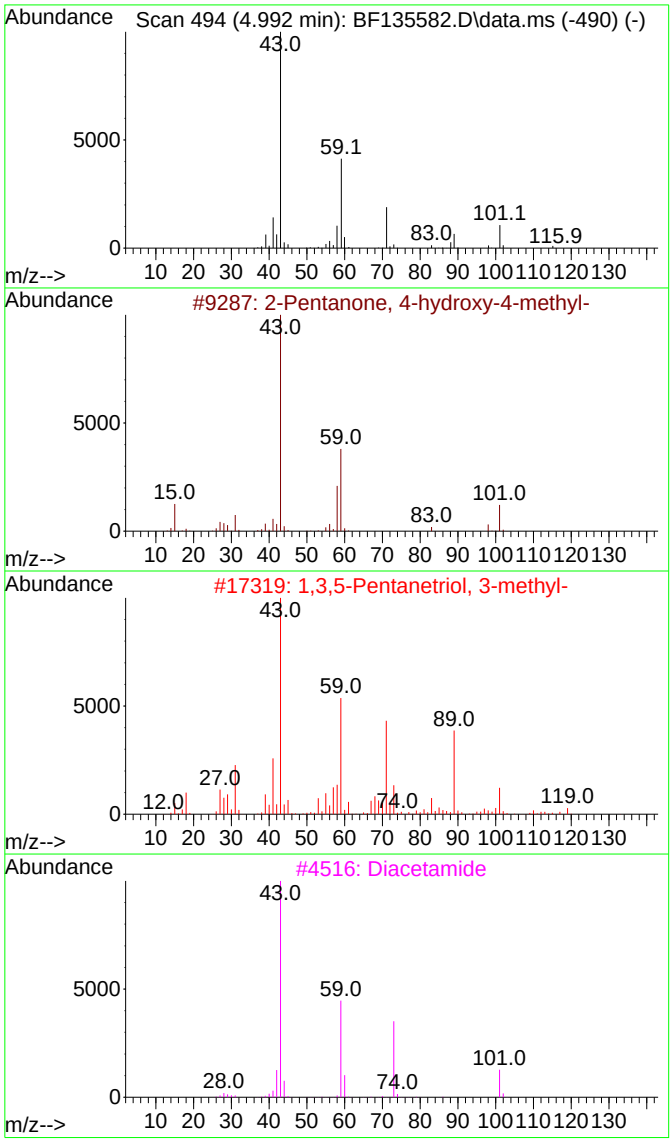
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

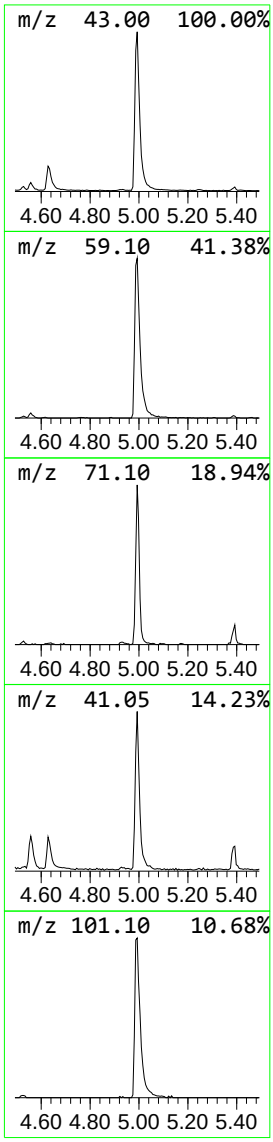
****

Peak Number 6 unknown4.992 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	15.44 ng	723978	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
3	Diacetamide	101	C4H7NO2	000625-77-4	33
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	14
5	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	9





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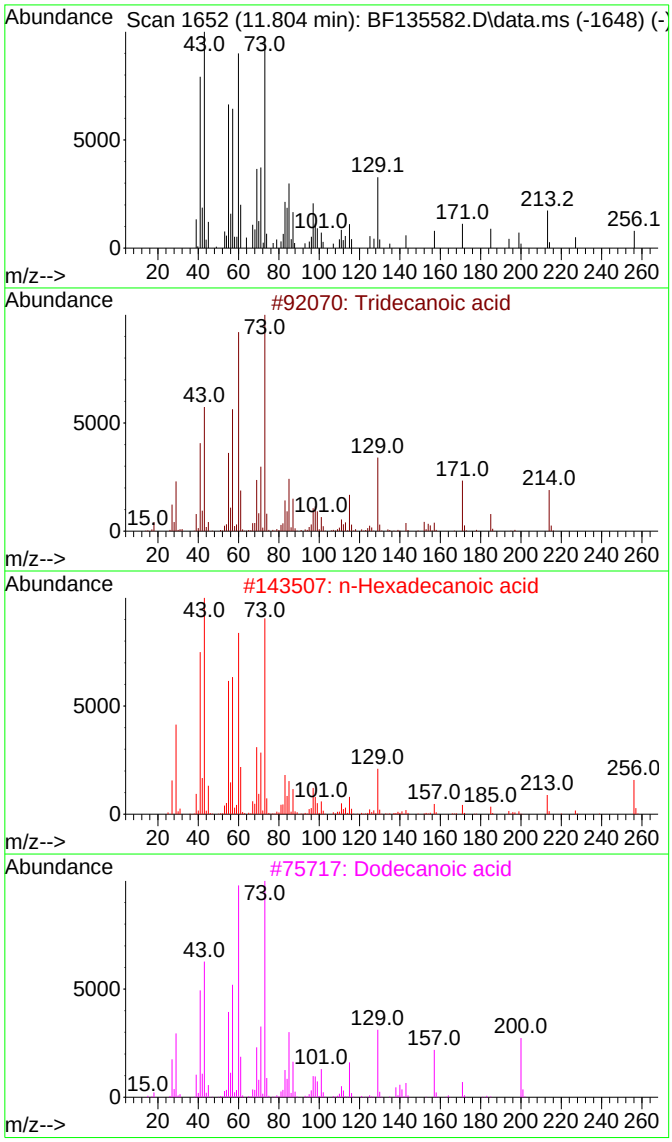
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

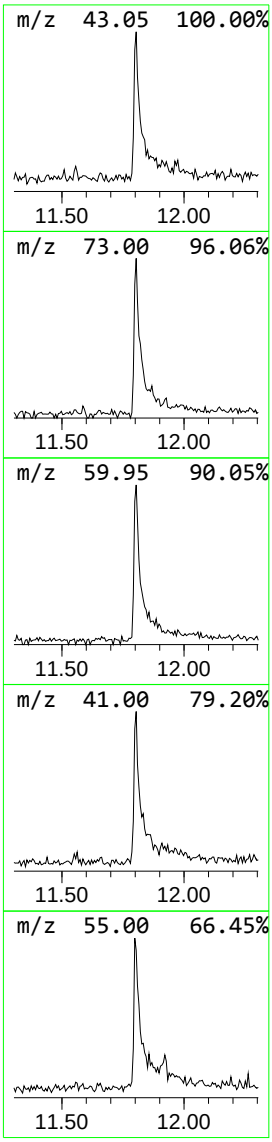
****

Peak Number 7 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	2.38 ng	169206	Phenanthrene-d10	11.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	81
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3	Dodecanoic acid	200	C12H24O2	000143-07-7	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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
n-Propyl acetate	2.722	9.2	ng	432138	1	6.739	937536	20.0
4-Penten-2-one,...	3.487	9.4	ng	438638	1	6.739	937536	20.0
3-Penten-2-one,...	4.363	49.6	ng	2324870	1	6.739	937536	20.0
Propanoic acid,...	4.557	2.3	ng	106522	1	6.739	937536	20.0
Cyclotrisiloxan...	4.616	5.0	ng	236043	1	6.739	937536	20.0
unknown4.992	4.992	15.4	ng	723978	1	6.739	937536	20.0
Tridecanoic acid	11.804	2.4	ng	169206	4	11.263	1421830	20.0