LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102523\
Data File : BF135945.D
Acq On : 25 Oct 2023 17:20
Operator : CG\JU
Sample : PB156430BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB156430BL

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-BF102523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135945.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	18	23	29	rVB	82057	112645	1.65%	0.238%
2	3.640	259	264	273	rVB	110194	156976	2.30%	0.332%
3	4.475	400	406	410	rBV	2367227	2708607	39.70%	5.724%
4	5.087	501	510	521	rBV	2319977	3862161	56.61%	8.162%
5	5.469	569	575	578	rBV	4836203	5935924	87.01%	12.544%
6	5.851	636	640	643	rBV	222419	171853	2.52%	0.363%
7	6.457	736	743	746	rBV	4461874	5852745	85.79%	12.368%
8	6.822	801	805	808	rBV	1202959	933263	13.68%	1.972%
9	7.387	894	901	904	rBV	3460424	3626706	53.16%	7.664%
10	8.098	1016	1022	1026	rBV	1492733	1308805	19.18%	2.766%
11	9.186	1199	1207	1210	rBV	6817813	6257839	91.73%	13.224%
12	9.857	1315	1321	1324	rBV	1880795	1476201	21.64%	3.120%
13	10.651	1451	1456	1459	rBV	4068328	3904691	57.24%	8.252%
14	11.351	1571	1575	1578	rBV	1767536	1532793	22.47%	3.239%
15	12.957	1842	1848	1851	rBV	6539002	6822097	100.00%	14.417%
16	14.004	2022	2026	2029	rBV	1437653	1351490	19.81%	2.856%
17	15.486	2272	2278	2287	rBV	900373	1119043	16.40%	2.365%
18	17.380	2588	2600	2620	rVB4	37240	186340	2.73%	0.394%

Sum of corrected areas: 47320179

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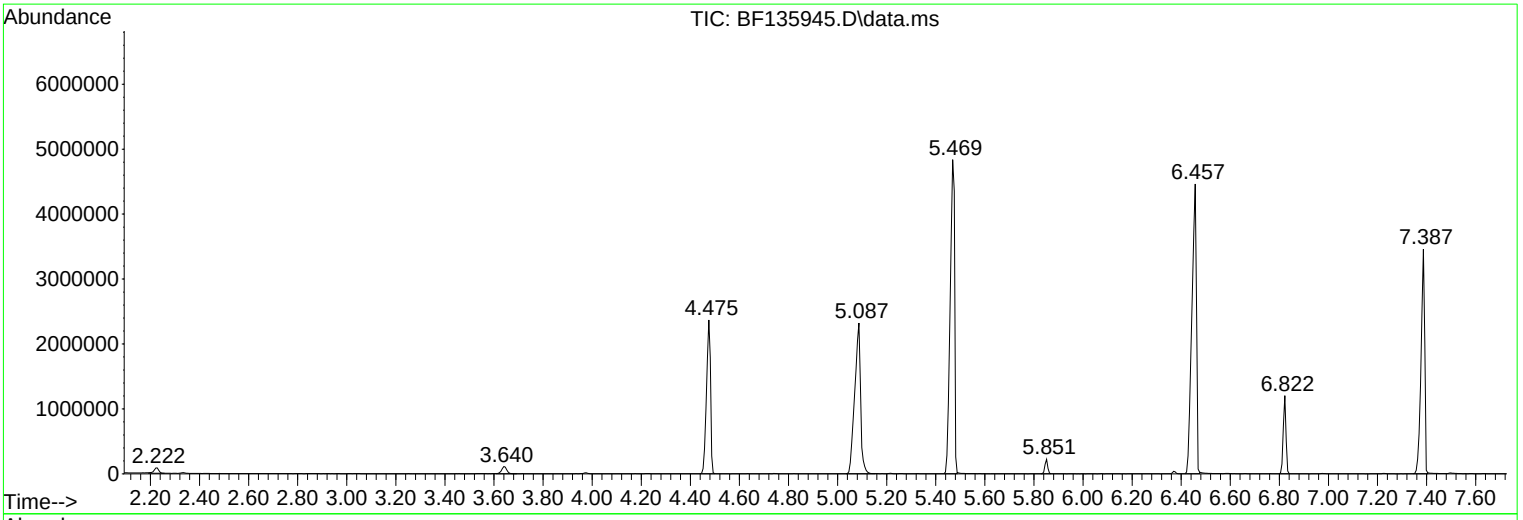
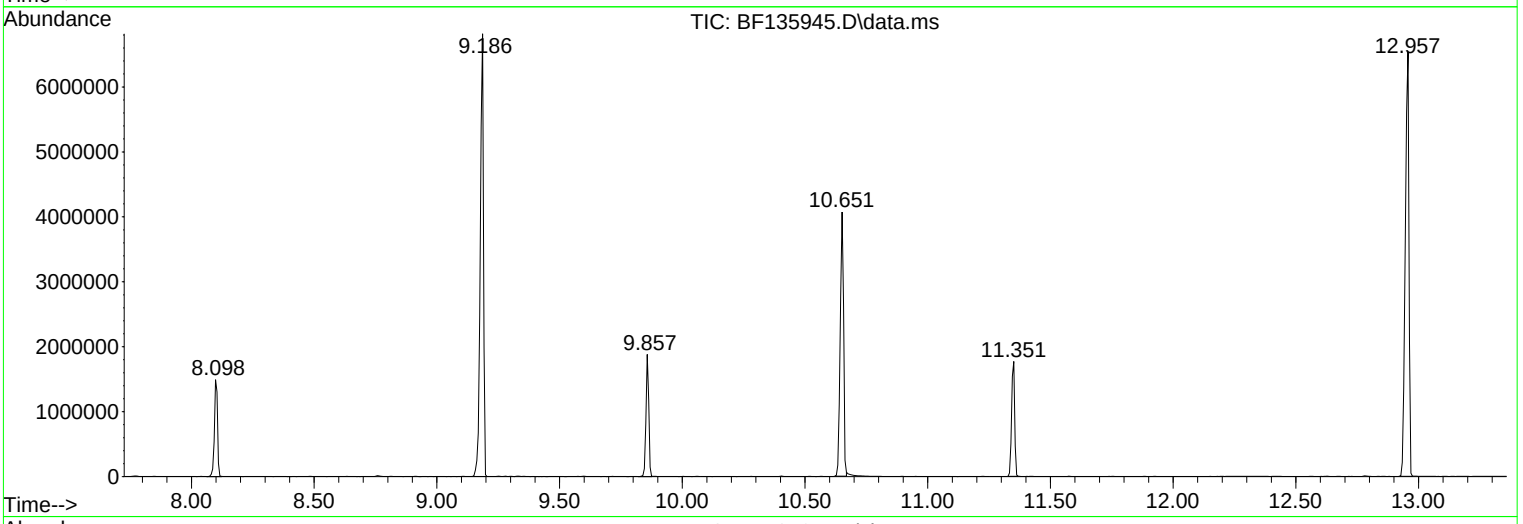
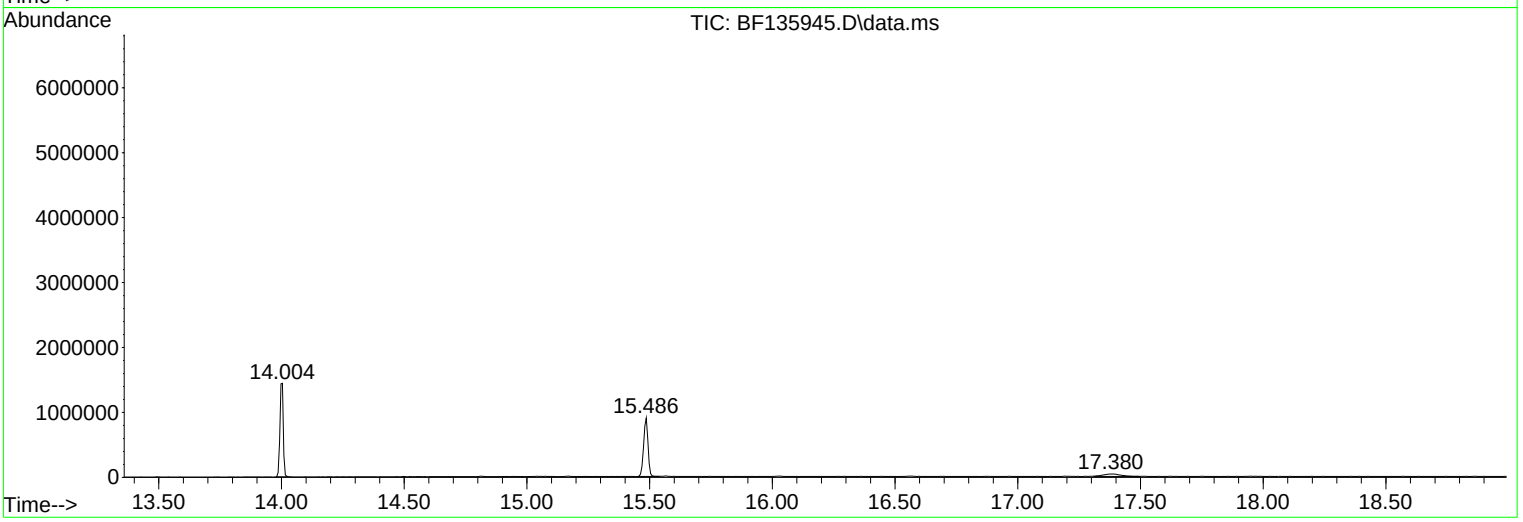
Instrument :
BNA_F
ClientSampleId :
PB156430BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.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

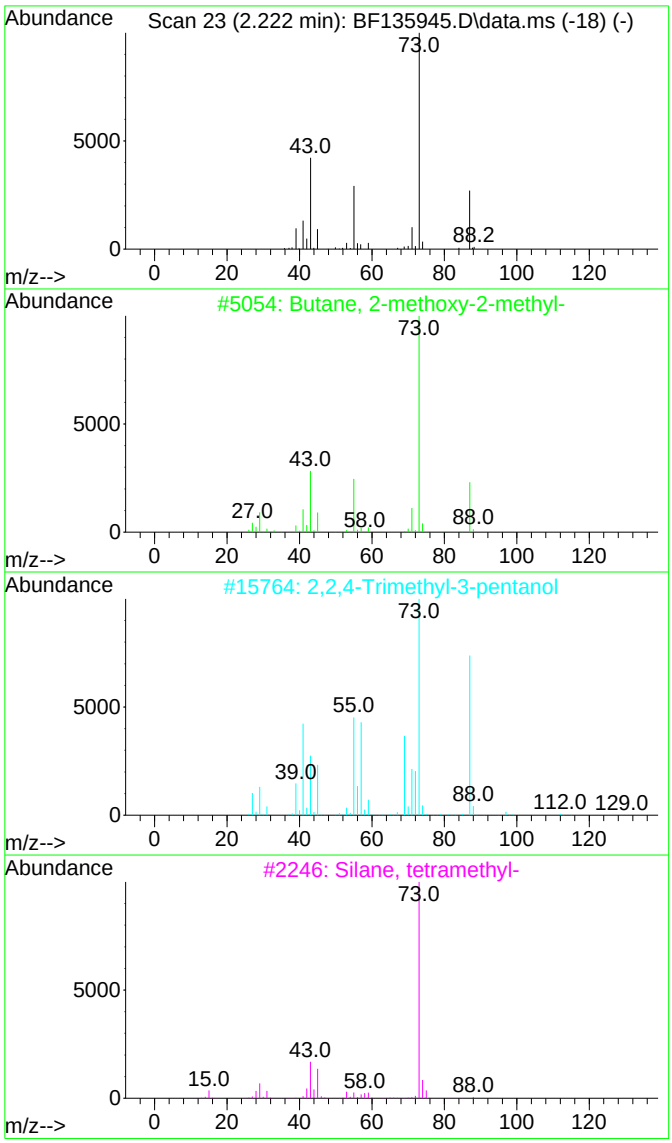
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

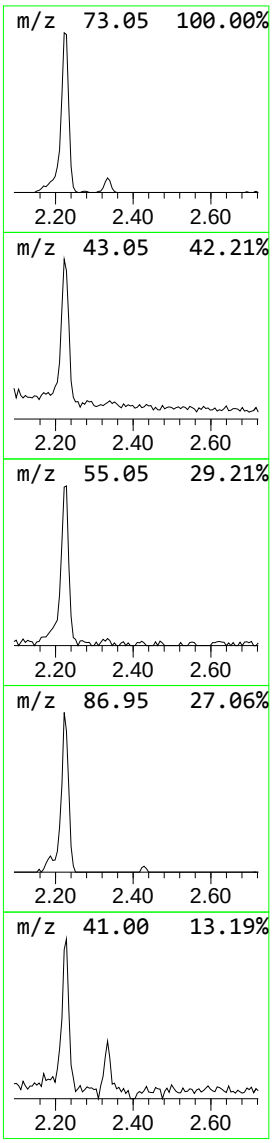
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	2.41 ng	112645	1,4-Dichlorobenzene-d4	6.822

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.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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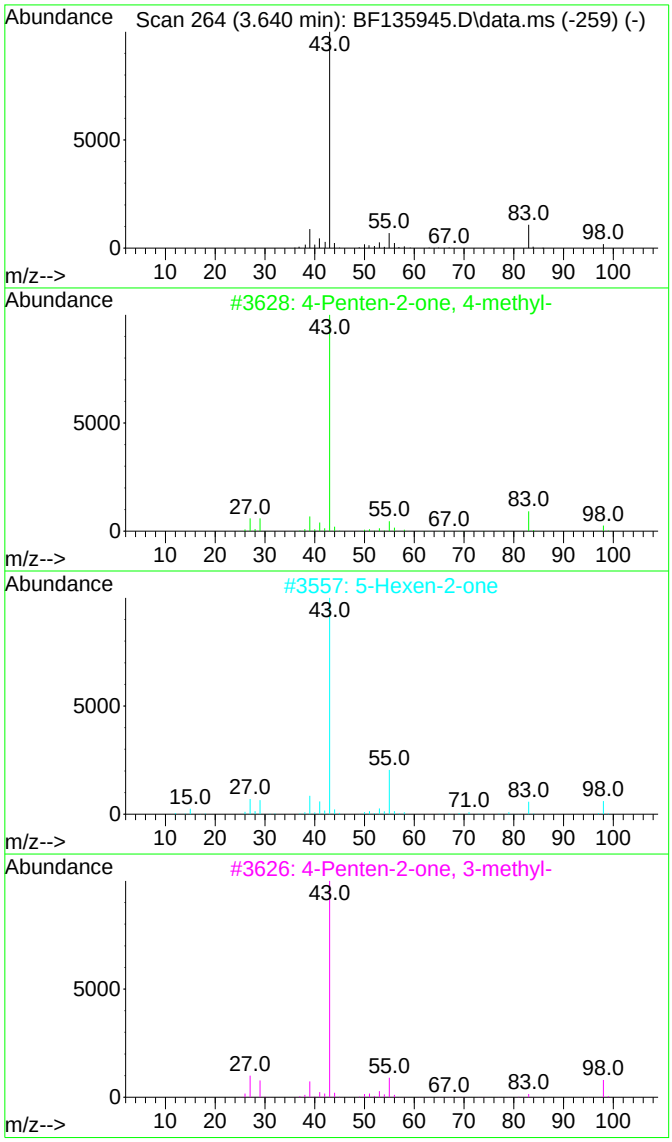
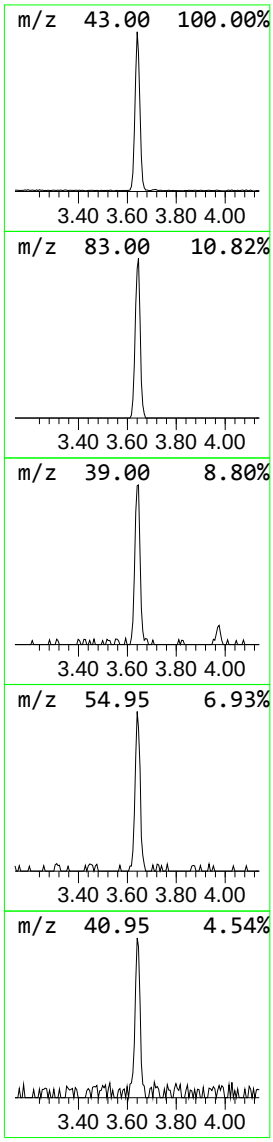
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.640	3.36 ng	156976	1,4-Dichlorobenzene-d4	6.822

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	37
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	33
4	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	28
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





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Data File : BF135945.D
Acq On : 25 Oct 2023 17:20
Operator : CG\JU
Sample : PB156430BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB156430BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

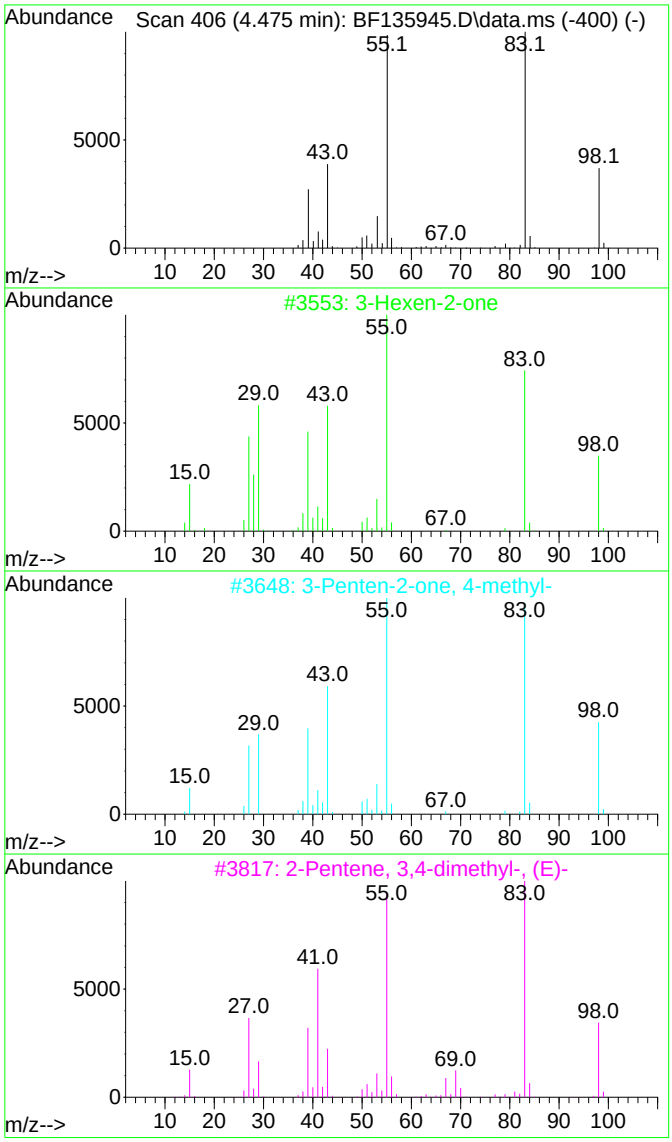
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

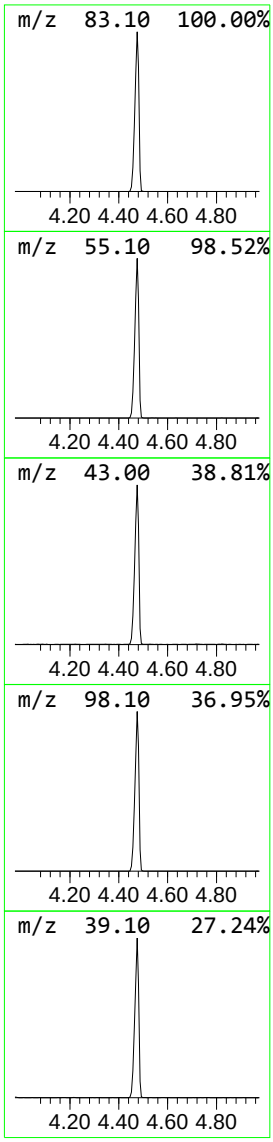
****

Peak Number 3 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.475	58.05 ng	2708610	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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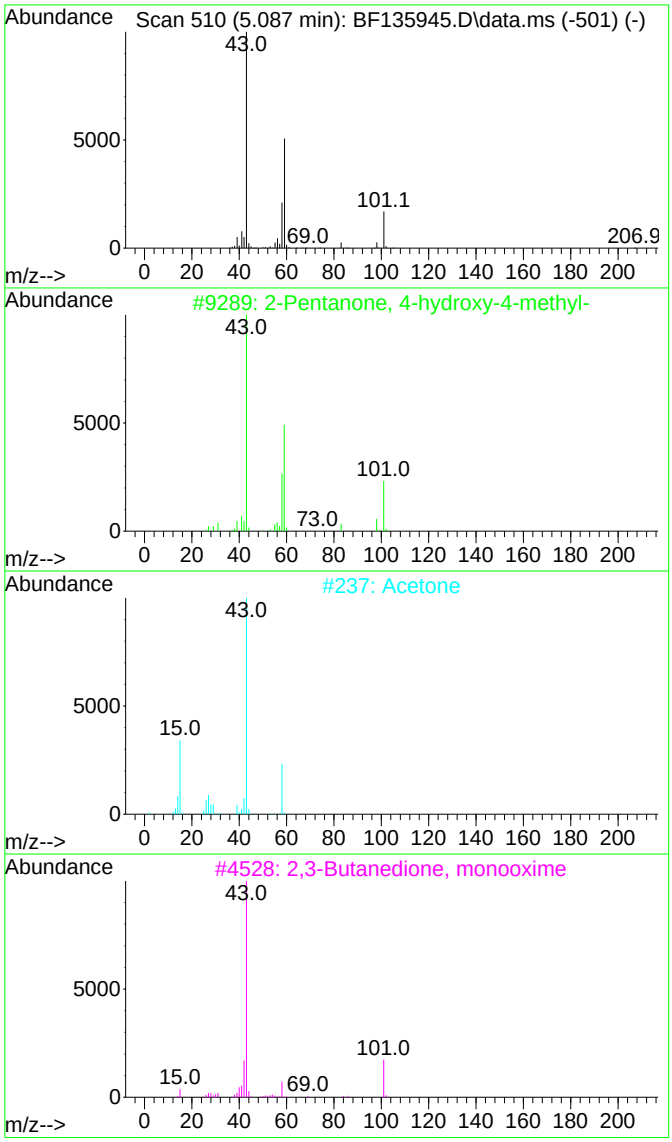
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

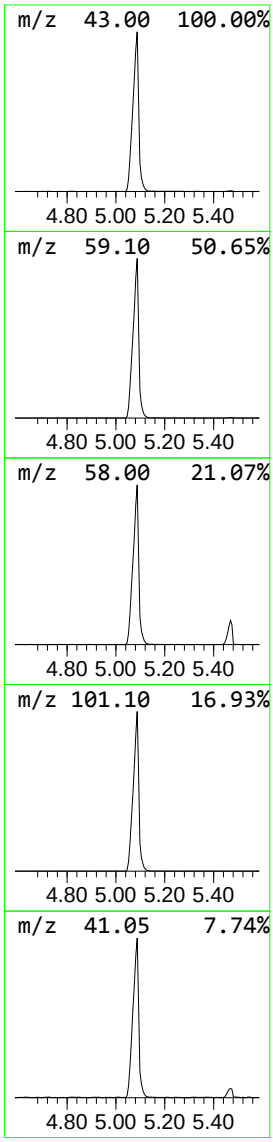
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	82.77 ng	3862160	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Acetone	58	C3H6O	000067-64-1	16
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9





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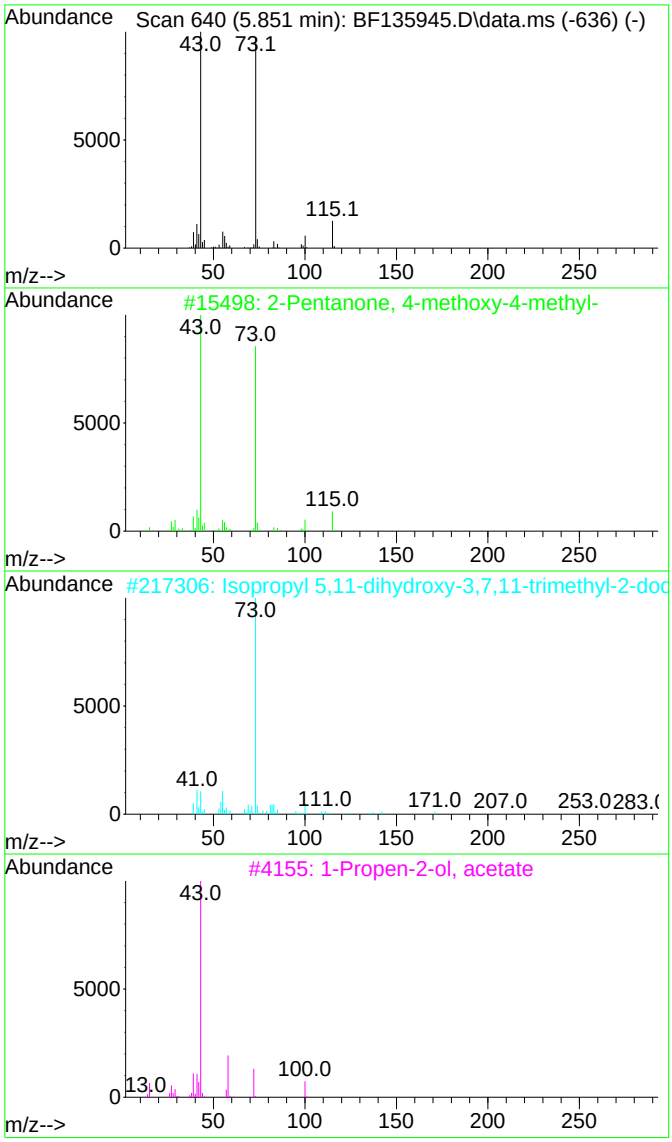
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

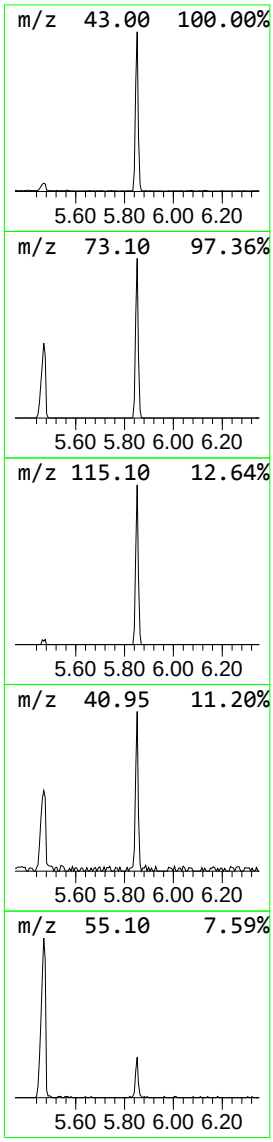
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.851	3.68 ng	171853	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Isopropyl 5,11-dihydroxy-3,7,11-...	314	C18H34O4	1000223-34-1	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





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TIC Library : C:\Database\NIST20.L
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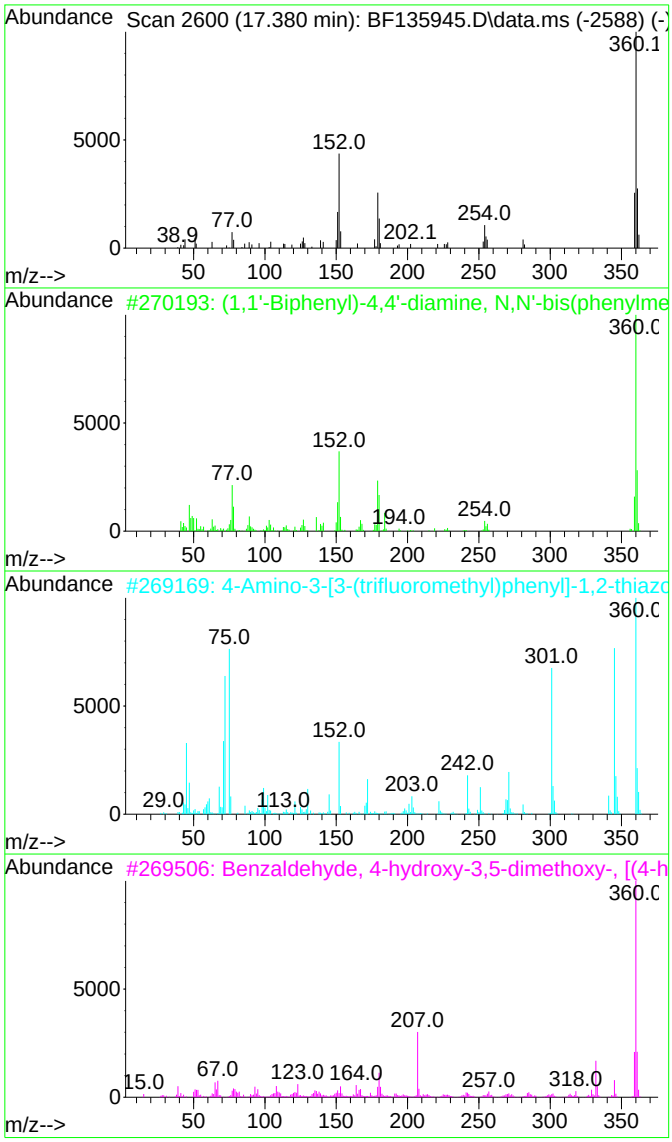
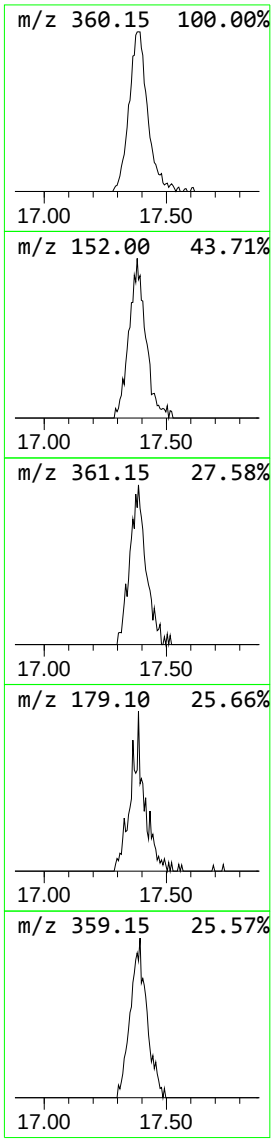
****
Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.380	3.33 ng	186340	Perylene-d12	15.486

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	91
2	4-Amino-3-[3-(trifluoromethyl)ph...	360	C14H15F3N2O2SSi	1010500-98-0	52
3	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	49
4	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
5	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	46





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
Butane, 2-metho...	2.222	2.4	ng	112645	1	6.822	933263	20.0
4-Penten-2-one,...	3.640	3.4	ng	156976	1	6.822	933263	20.0
3-Hexen-2-one	4.475	58.0	ng	2708610	1	6.822	933263	20.0
2-Pentanone, 4-...	5.087	82.8	ng	3862160	1	6.822	933263	20.0
2-Pentanone, 4-...	5.851	3.7	ng	171853	1	6.822	933263	20.0
(1,1'-Biphenyl)...	17.380	3.3	ng	186340	6	15.486	1119040	20.0