LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111023\
Data File : BM042695.D
Acq On : 10 Nov 2023 17:22
Operator : MA/JU
Sample : 05317-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
208

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_M\Methods\8270-BM103023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.381	401	407	421	rBV	581228	878610	62.36%	7.737%
2	6.445	583	588	595	rVB	23090	36394	2.58%	0.320%
3	7.016	678	685	694	rBV	567209	943331	66.96%	8.306%
4	7.845	817	826	837	rBV	368912	603538	42.84%	5.314%
5	9.045	1023	1030	1044	rBV	357182	627299	44.53%	5.524%
6	10.663	1298	1305	1312	rBV	445620	739349	52.48%	6.510%
7	12.063	1537	1543	1547	rBV7	21095	48984	3.48%	0.431%
8	12.198	1561	1566	1568	rBV4	20669	36530	2.59%	0.322%
9	12.410	1599	1602	1607	rBV2	28005	45283	3.21%	0.399%
10	12.551	1623	1626	1631	rVB3	35626	48462	3.44%	0.427%
11	12.645	1637	1642	1649	rVB8	40505	86366	6.13%	0.760%
12	12.710	1649	1653	1657	rBV6	25224	50353	3.57%	0.443%
13	12.810	1666	1670	1674	rBV6	39868	66259	4.70%	0.583%
14	13.039	1705	1709	1717	rVB2	71422	123956	8.80%	1.091%
15	13.121	1718	1723	1728	rBV	965044	1408848	100.00%	12.406%
16	13.598	1800	1804	1808	rBV2	115360	174224	12.37%	1.534%
17	13.980	1866	1869	1876	rVB3	266293	449786	31.93%	3.961%
18	14.121	1890	1893	1899	rVB4	292088	434041	30.81%	3.822%
19	14.186	1900	1904	1908	rBV2	237432	410546	29.14%	3.615%
20	14.510	1955	1959	1963	rBV	570306	791676	56.19%	6.971%
21	15.245	2081	2084	2089	rVB2	701164	838089	59.49%	7.380%
22	19.880	2869	2872	2876	rBV	888128	1066705	75.71%	9.393%
23	22.715	3351	3354	3359	rVB	260304	321554	22.82%	2.831%
24	23.062	3409	3413	3415	rBV2	332547	526315	37.36%	4.634%
25	23.821	3538	3542	3548	rVB	346680	600064	42.59%	5.284%

Sum of corrected areas: 11356562

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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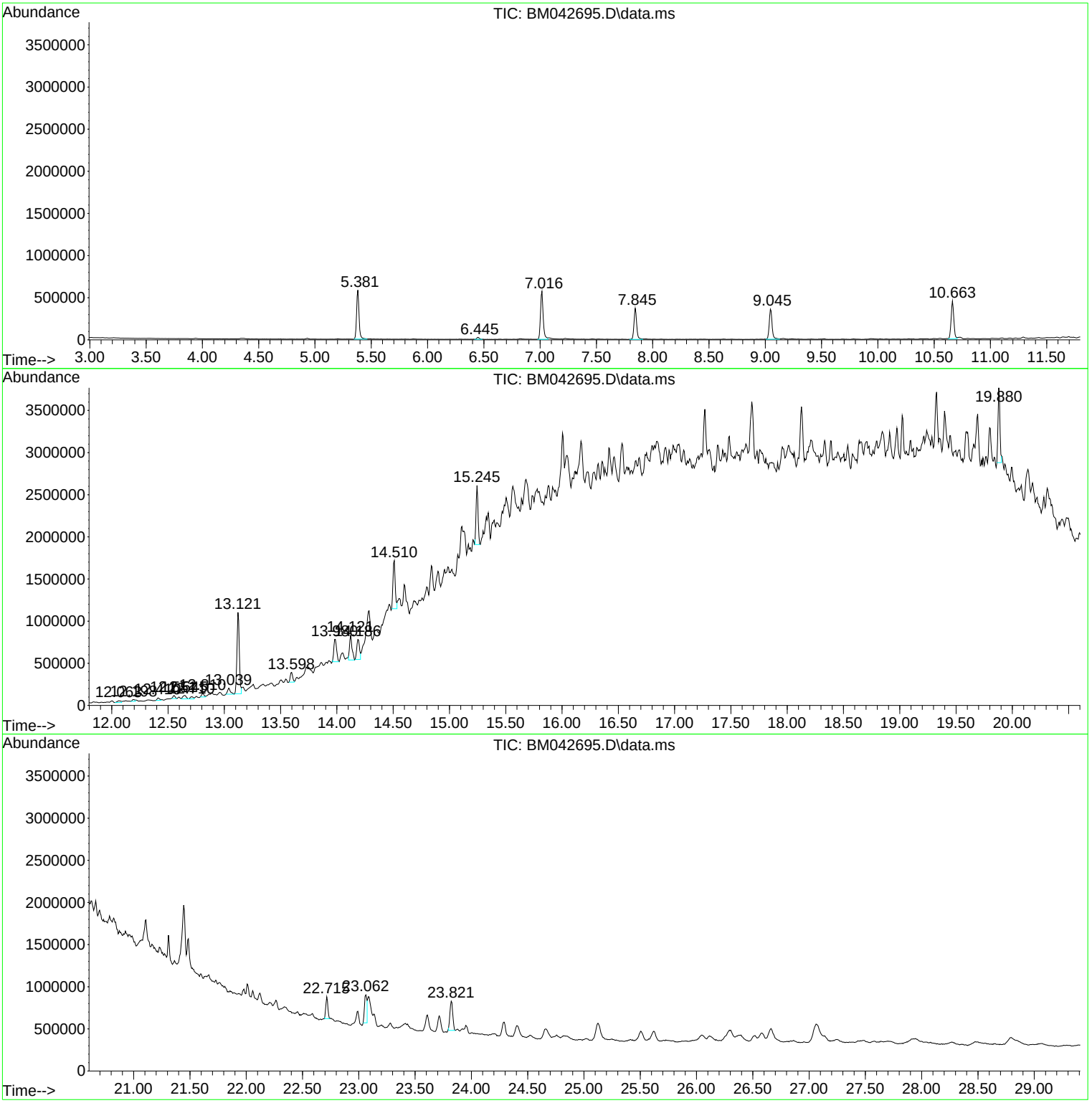
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM042695.D
Acq On : 10 Nov 2023 17:22
Operator : MA/JU
Sample : 05317-01 2X
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

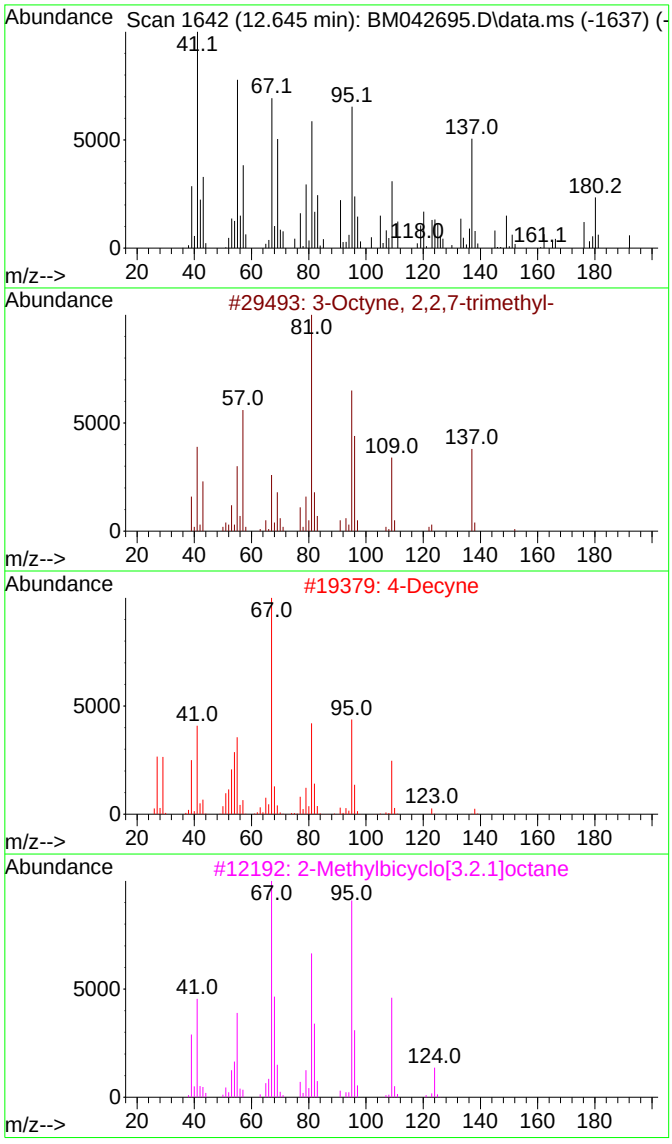
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

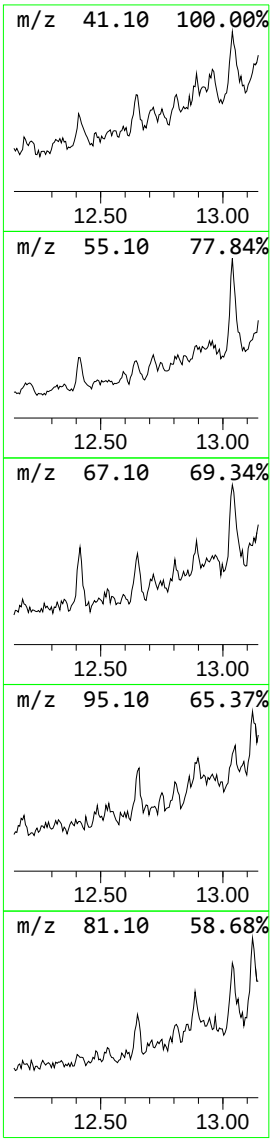
****

Peak Number 1 3-Octyne, 2,2,7-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.18 ng	86366	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	52
2	4-Decyne	138	C10H18	002384-86-3	50
3	2-Methylbicyclo[3.2.1]octane	124	C9H16	1010215-28-0	49
4	cis,trans-2-Ethylbicyclo[4.4.0]d...	166	C12H22	066660-38-6	46
5	trans,trans-2,8-Dimethylspiro[5....	180	C13H24	095530-76-0	43





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Data File : BM042695.D
Acq On : 10 Nov 2023 17:22
Operator : MA/JU
Sample : 05317-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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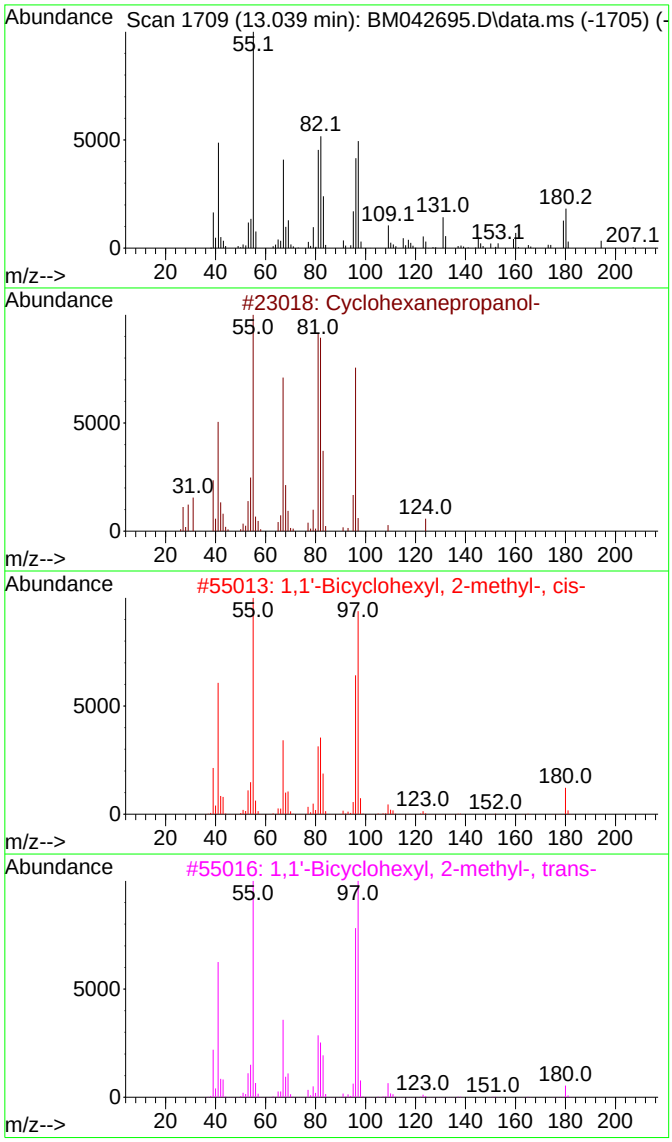
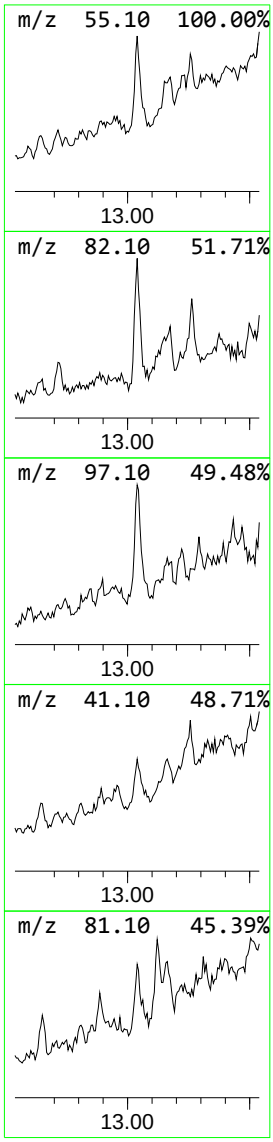
Peak Number 2 Cyclohexanepropanol- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.039	3.13 ng	123956	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanepropanol-	142	C9H18O	001124-63-6	52
2	1,1'-Bicyclohexyl, 2-methyl-, cis-	180	C13H24	050991-08-7	47
3	1,1'-Bicyclohexyl, 2-methyl-, tr...	180	C13H24	050991-09-8	43
4	E-1,9-Tetradecadiene	194	C14H26	1000245-70-7	41
5	Acetic acid, trifluoro-, cyclohe...	196	C8H11F3O2	001549-45-7	35





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Data File : BM042695.D
Acq On : 10 Nov 2023 17:22
Operator : MA/JU
Sample : 05317-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
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TIC Library : C:\Database\NIST20.L
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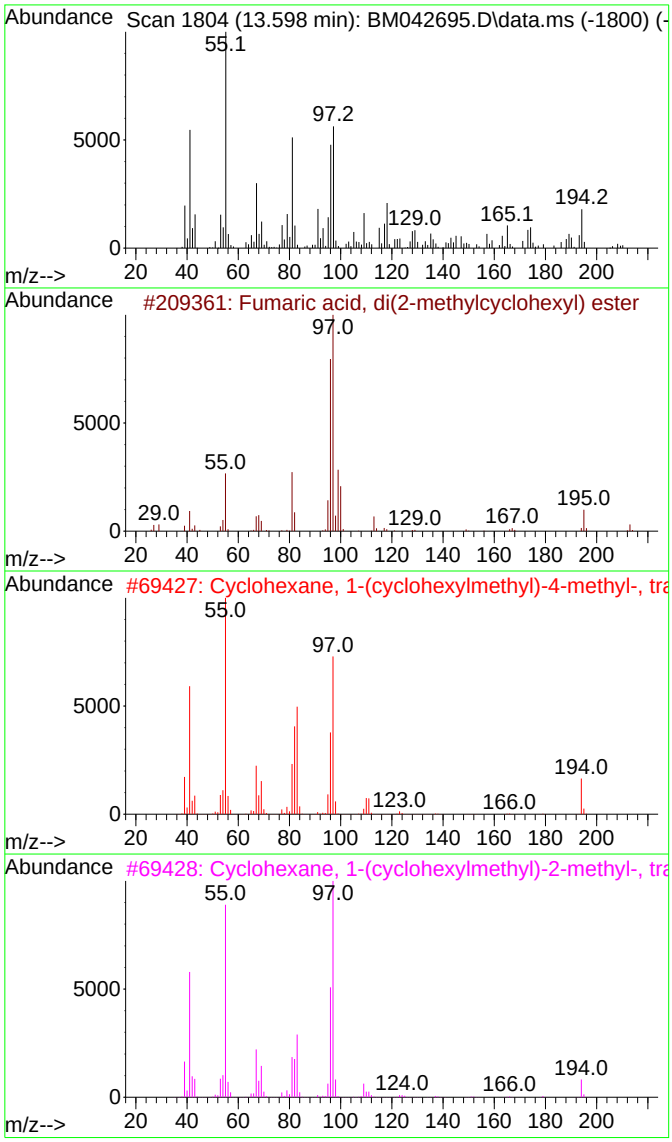
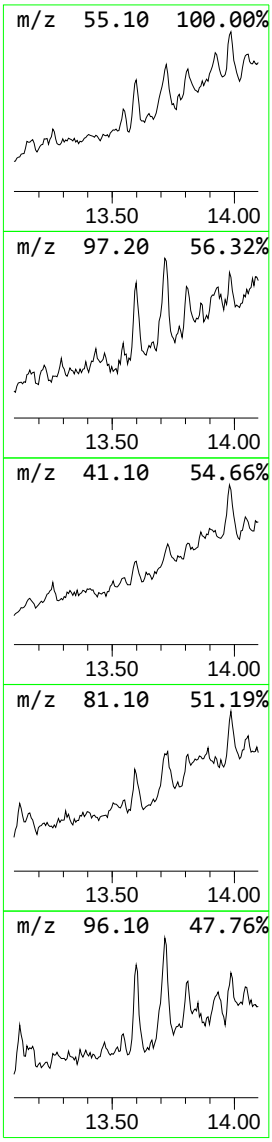
****

Peak Number 3 unknown13.598 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.598	4.40 ng	174224	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, di(2-methylcyclohe...	308	C18H28O4	1000345-10-9	43
2	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-98-2	38
3	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-94-8	35
4	1-Methylcyclooctene	124	C9H16	000933-11-9	27
5	Cyclohexane, 1-(cyclohexylmethyl...	194	C14H26	054823-96-0	27





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Data File : BM042695.D
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
208

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

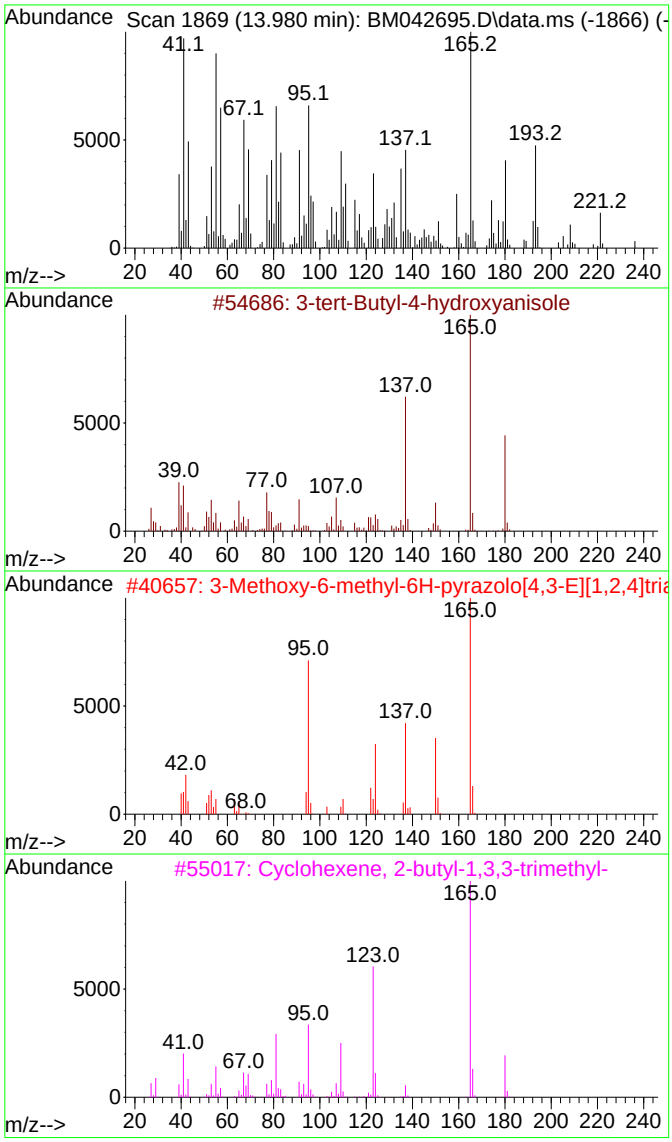
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

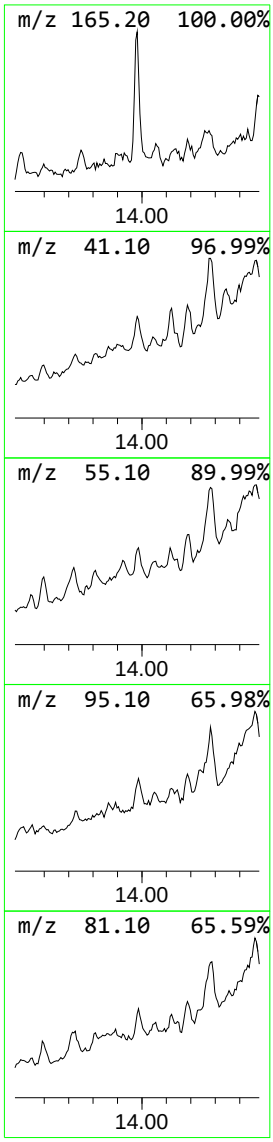
****

Peak Number 4 3-tert-Butyl-4-hydroxyanisole Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	11.36 ng	449786	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	64
2	3-Methoxy-6-methyl-6H-pyrazolo[4...	165	C6H7N5O	037526-57-1	50
3	Cyclohexene, 2-butyl-1,3,3-trime...	180	C13H24	003293-50-3	49
4	7-Methyl-8-oxo-1,2,3,4-tetrahydr...	165	C8H11N3O	026955-10-2	38
5	9H-Fluorene, 9-methyl-	180	C14H12	002523-37-7	38





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Data File : BM042695.D
Acq On : 10 Nov 2023 17:22
Operator : MA/JU
Sample : 05317-01 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
208

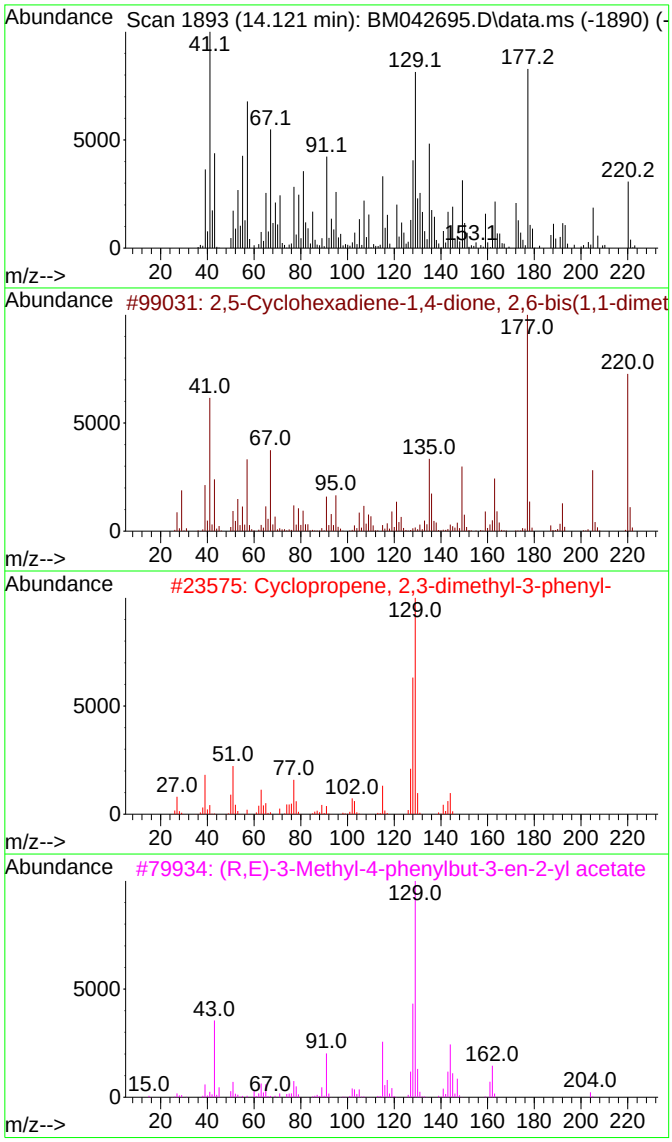
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

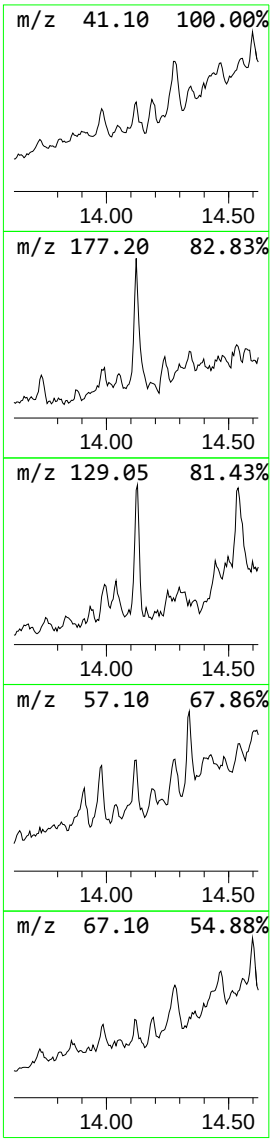
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	10.97 ng	434041	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	90
2	Cyclopropene, 2,3-dimethyl-3-phe...	144	C11H12	1000162-49-5	30
3	(R,E)-3-Methyl-4-phenylbut-3-en-...	204	C13H16O2	187735-90-6	25
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	144	C11H12	071721-26-1	25
5	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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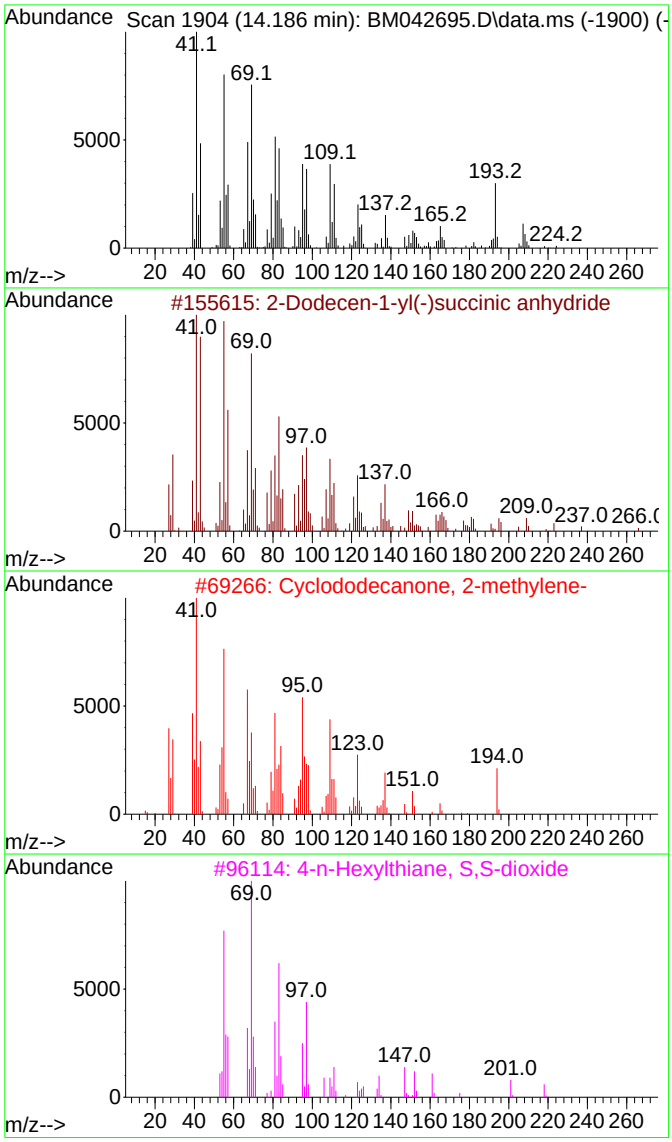
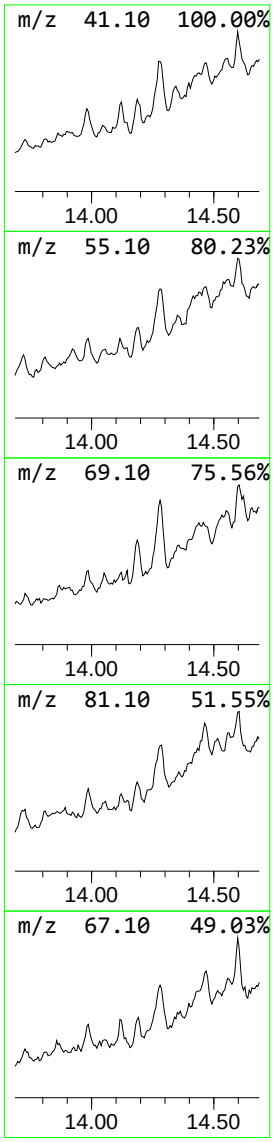
****
Peak Number 6 2-Dodecen-1-yl(-)succinic a... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.186	10.37 ng	410546	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	53
2	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	50
3	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	50
4	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	43
5	Pentanoic acid, 10-undecenyl ester	254	C16H30O2	1000159-93-4	43





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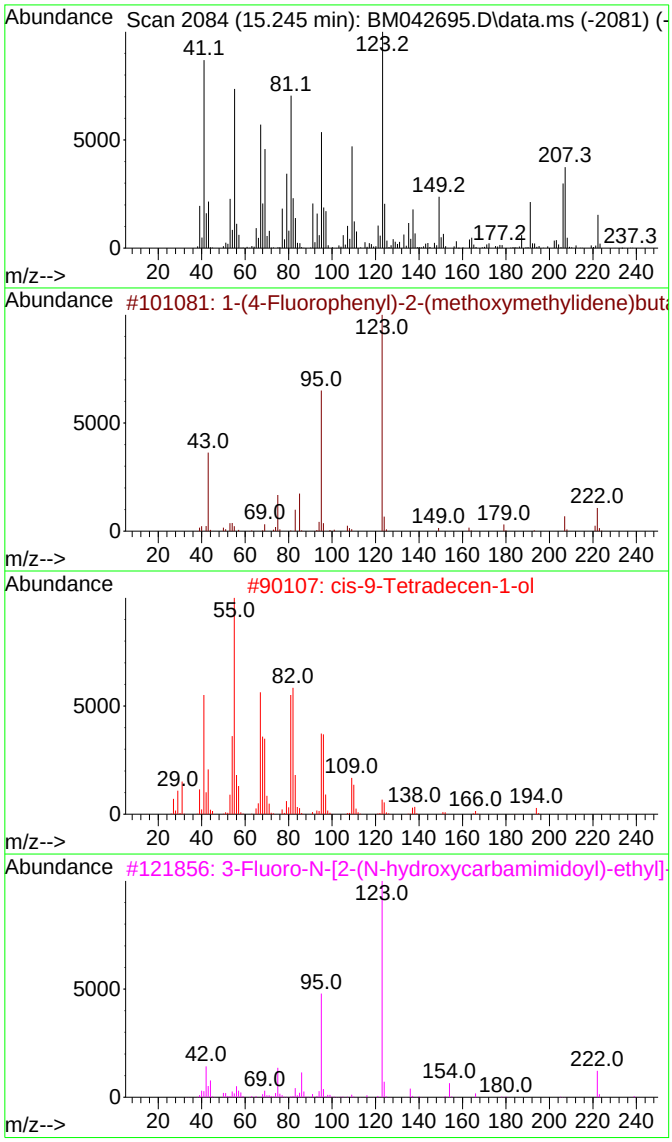
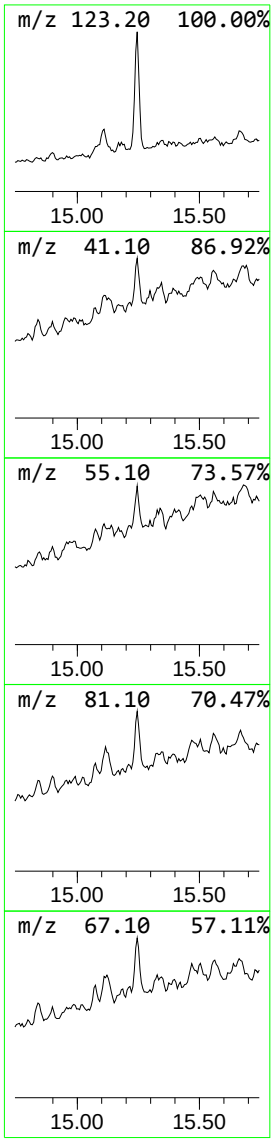
****

Peak Number 7 unknown15.245 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.245	21.17 ng	838089	Acenaphthene-d10	14.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	38
2	cis-9-Tetradecen-1-ol	212	C14H28O	035153-15-2	38
3	3-Fluoro-N-[2-(N-hydroxycarbamim...	239	C11H14FN3O2	1010297-41-5	35
4	Cyclohexanone, 2-(1-methyl-2-nit...	185	C9H15NO3	019307-62-1	35
5	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	35





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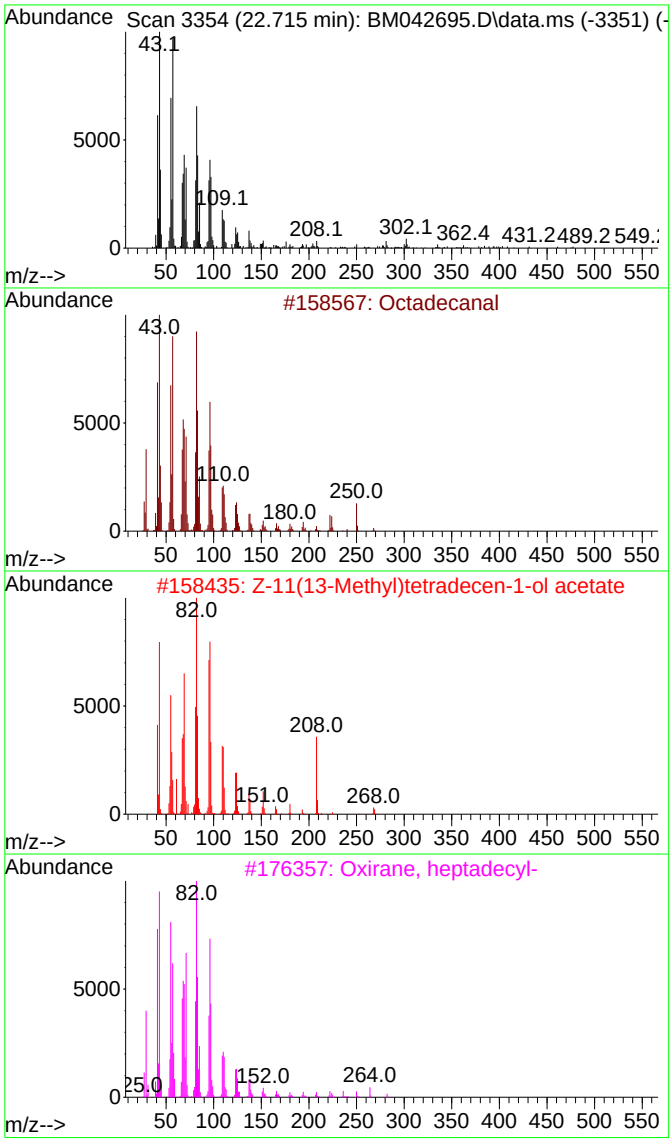
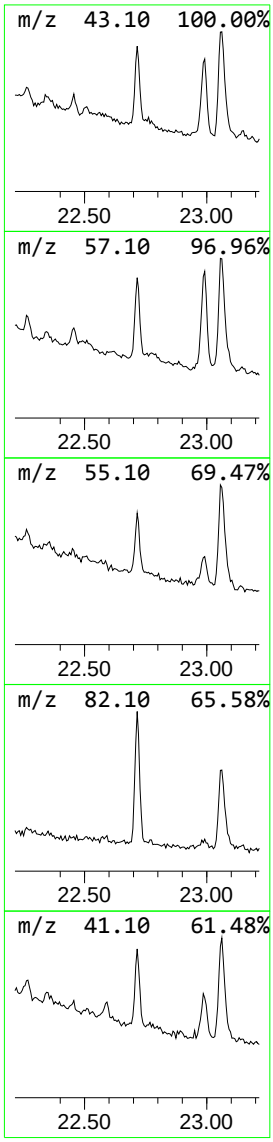
Peak Number 8 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.715	10.72 ng	321554	Perylene-d12	23.821

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	94
2	Z-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000131-33-3	93
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
4	Henicosanal	310	C21H42O	051227-32-8	93
5	11-Eicosenol	296	C20H40O	1010424-20-3	91





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
3-Octyne, 2,2,7...	12.645	2.2	ng	86366	3	14.510	791676	20.0
Cyclohexaneprop...	13.039	3.1	ng	123956	3	14.510	791676	20.0
unknown13.598	13.598	4.4	ng	174224	3	14.510	791676	20.0
3-tert-Butyl-4-...	13.980	11.4	ng	449786	3	14.510	791676	20.0
2,5-Cyclohexadi...	14.121	11.0	ng	434041	3	14.510	791676	20.0
2-Dodecen-1-yl(...	14.186	10.4	ng	410546	3	14.510	791676	20.0
unknown15.245	15.245	21.2	ng	838089	3	14.510	791676	20.0
Octadecanal	22.715	10.7	ng	321554	6	23.821	600064	20.0