LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003759.D
Acq On : 27 Oct 2020 17:39
Operator : CG/JU
Sample : L4523-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CS-42

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_P\METHODS\8270-BP101920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003759.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.093	30	35	55	rVB	5875362	7679784	93.86%	16.504%
2	3.252	55	62	73	rBV3	78582	185415	2.27%	0.398%
3	3.346	73	78	84	rBV	249862	351576	4.30%	0.756%
4	5.481	435	441	448	rVB	117135	171208	2.09%	0.368%
5	6.011	523	531	544	rBV	2071581	3093697	37.81%	6.648%
6	7.663	803	812	824	rBV	1947255	3200052	39.11%	6.877%
7	8.510	947	956	963	rBV	667378	1056233	12.91%	2.270%
8	9.675	1145	1154	1165	rBV	1339379	2209505	27.00%	4.748%
9	11.351	1430	1439	1447	rBV	814516	1383774	16.91%	2.974%
10	13.740	1836	1845	1853	rBV	3763468	5348445	65.37%	11.494%
11	14.528	1972	1979	1987	rBV	308792	423183	5.17%	0.909%
12	15.110	2071	2078	2087	rVB2	1316186	1929694	23.58%	4.147%
13	16.581	2321	2328	2343	rBV	2711841	3949224	48.26%	8.487%
14	17.828	2534	2540	2547	rBV	1600794	2332097	28.50%	5.012%
15	18.639	2674	2678	2686	rBV	86518	118893	1.45%	0.256%
16	20.304	2955	2961	2966	rBV	6560309	8182426	100.00%	17.584%
17	21.474	3156	3160	3170	rBV	448088	556303	6.80%	1.196%
18	21.845	3218	3223	3229	rVB	1727372	2354464	28.77%	5.060%
19	24.421	3653	3661	3670	rBV	947519	2006449	24.52%	4.312%

Sum of corrected areas: 46532422

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Misc :
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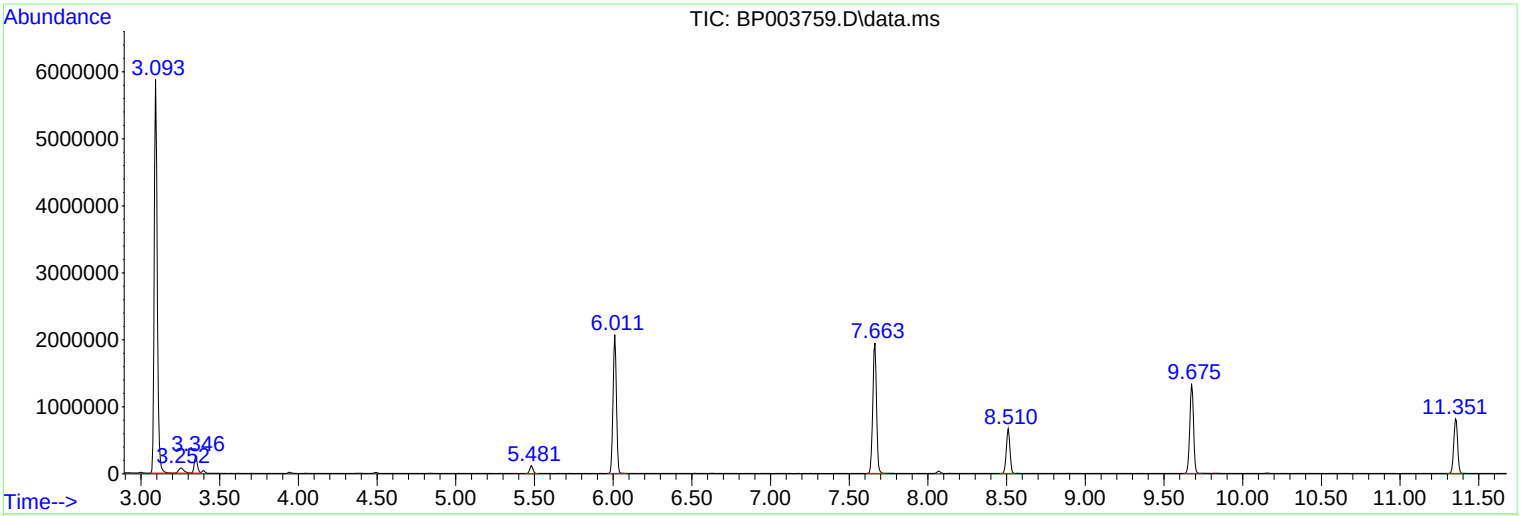
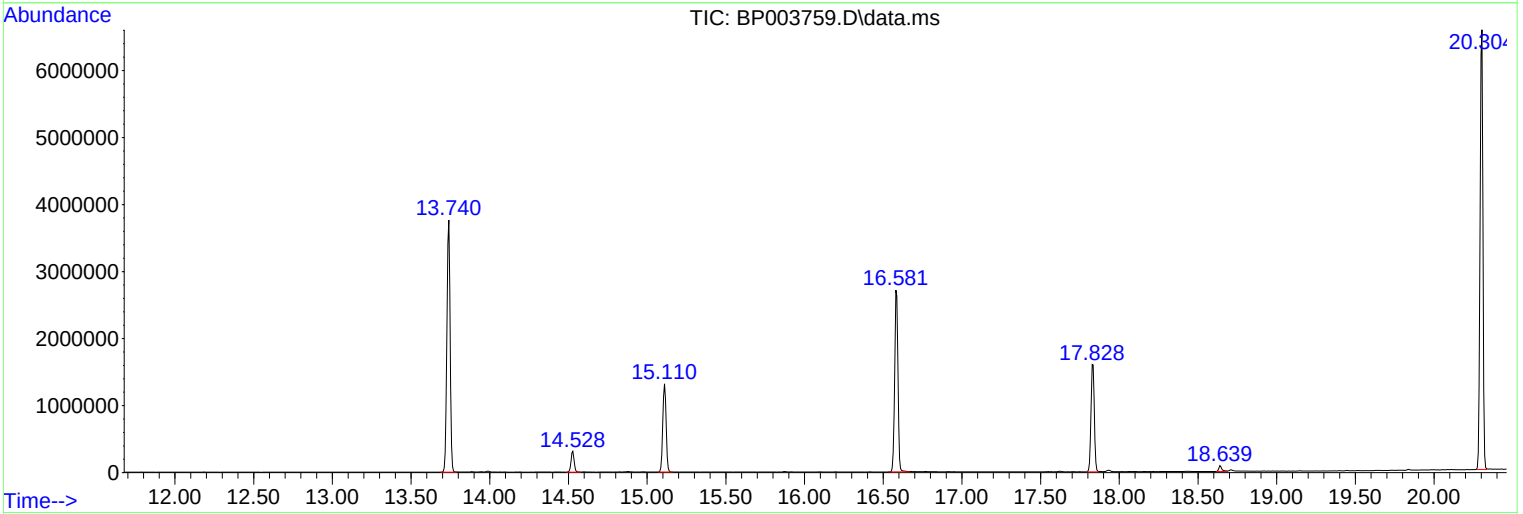
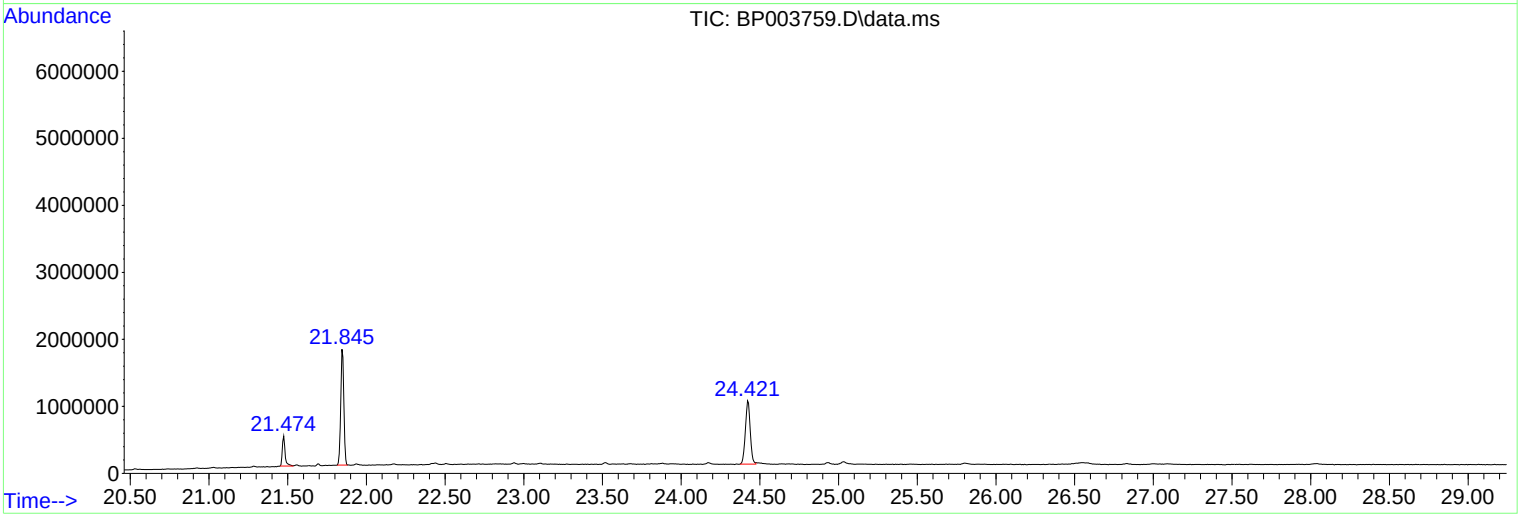
Instrument :
BNA_P
ClientSampleId :
CS-42

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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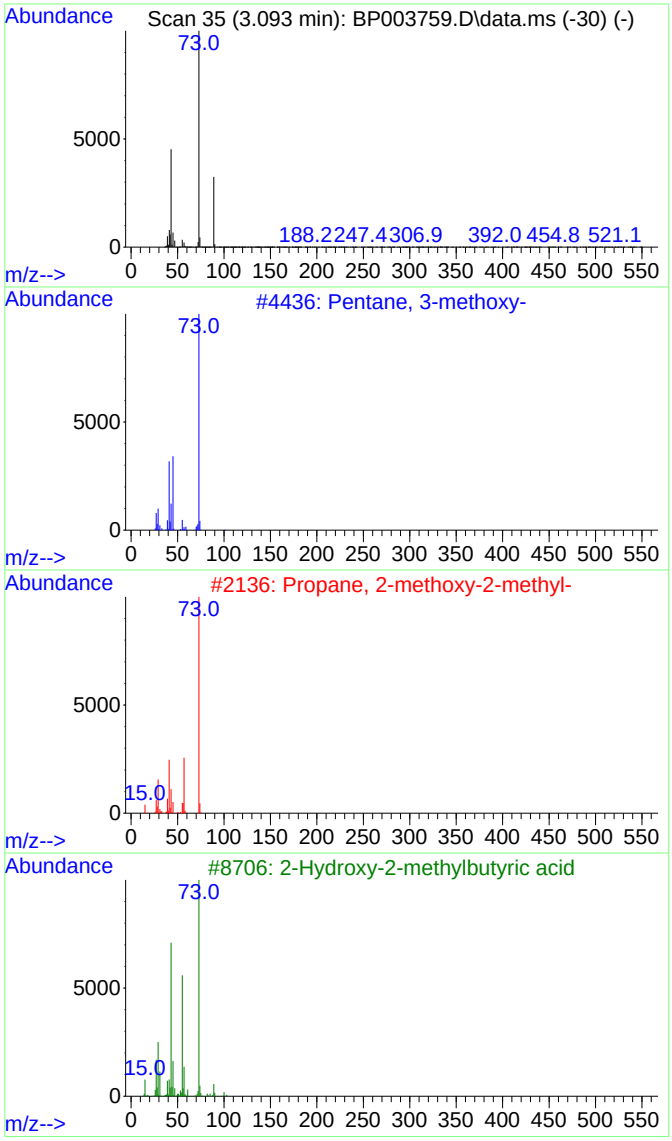
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

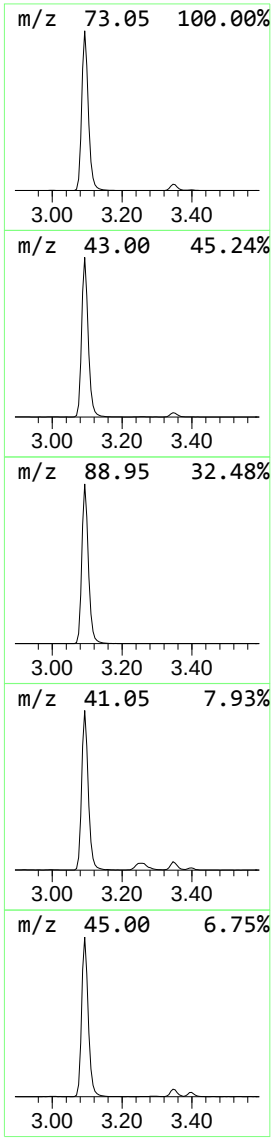
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown3.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.093	145.42 ng	7679780	1,4-Dichlorobenzene-d4	8.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	9
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7





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Sample : L4523-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CS-42

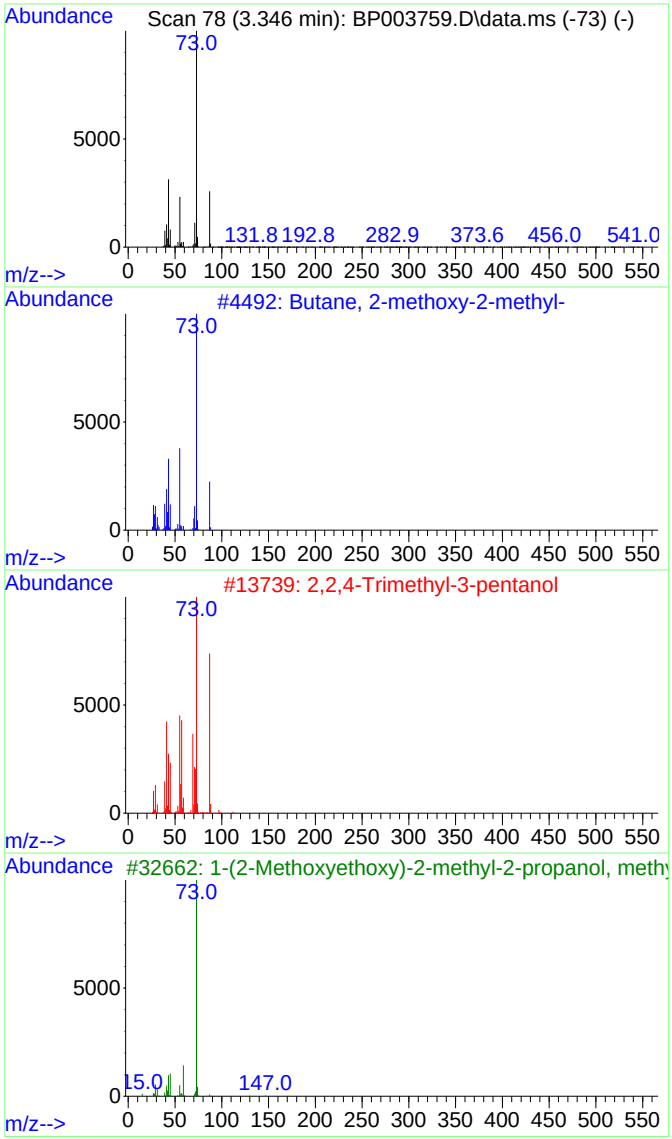
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

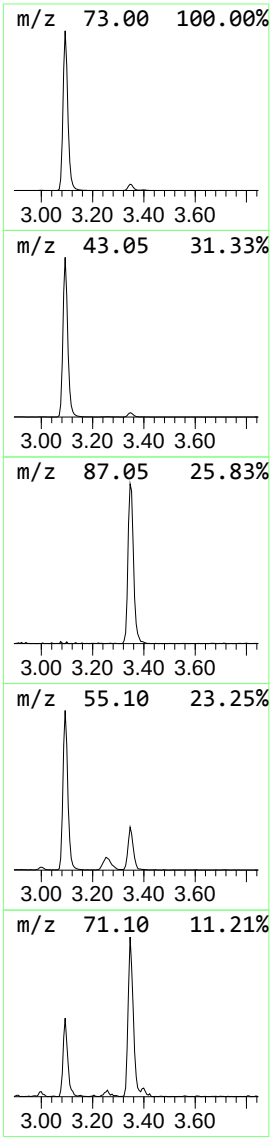
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.346	6.66 ng	351576	1,4-Dichlorobenzene-d4	8.510

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	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP102720\
Data File : BP003759.D
Acq On : 27 Oct 2020 17:39
Operator : CG/JU
Sample : L4523-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CS-42

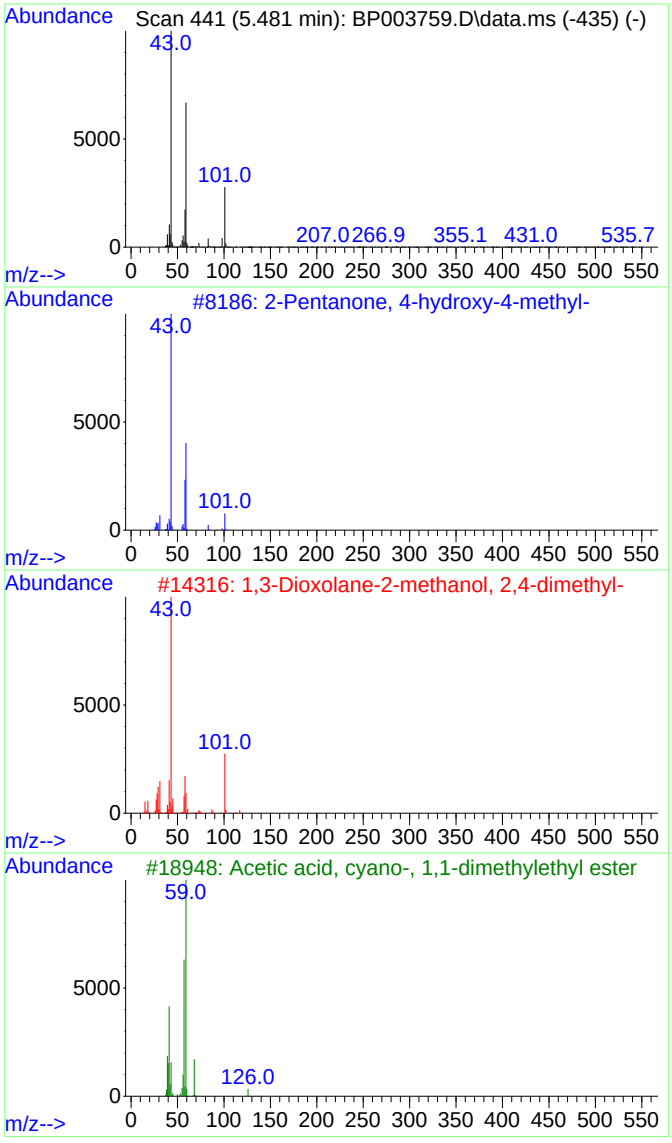
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

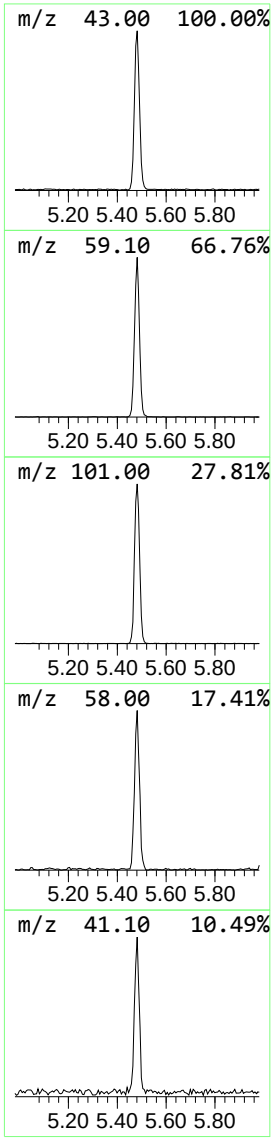
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.481	3.24 ng	171208	1,4-Dichlorobenzene-d4	8.510

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	16
5	Acetone	58	C3H6O	000067-64-1	10





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Sample : L4523-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CS-42

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101920.M
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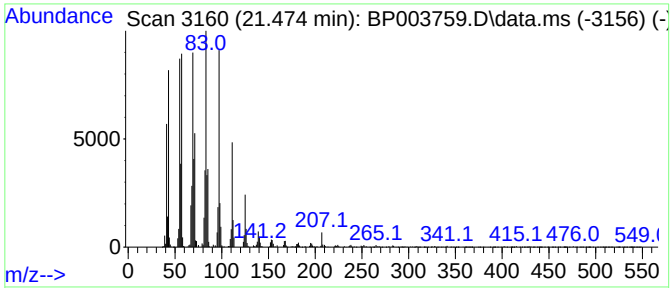
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

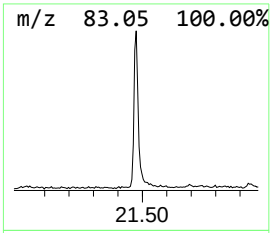
****

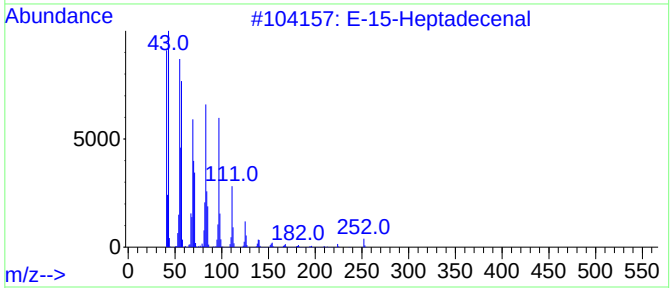
Peak Number 5 E-15-Heptadecenal Concentration Rank 3

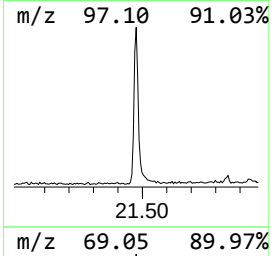
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.474	4.73 ng	556303	Chrysene-d12	21.845

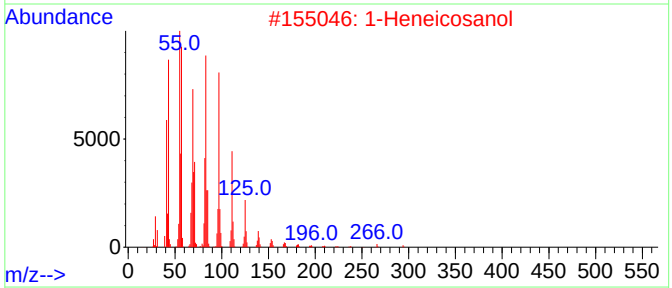
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94

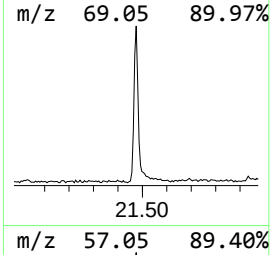


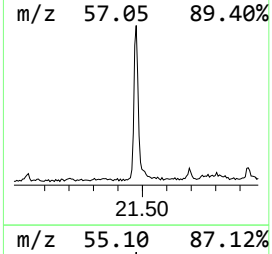


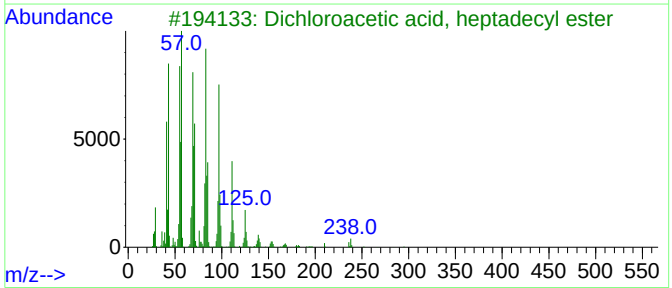


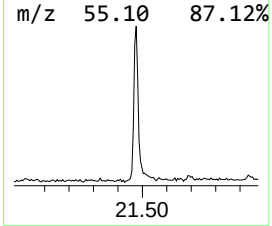












Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.09	3.093	145.4	ng	7679780	1	8.510	1056230	20.0
Butane, 2-metho...	3.346	6.7	ng	351576	1	8.510	1056230	20.0
2-Pentanone, 4-...	5.481	3.2	ng	171208	1	8.510	1056230	20.0
E-15-Heptadecenal	21.474	4.7	ng	556303	5	21.845	2354460	20.0