LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP101520\
Data File : BP003629.D
Acq On : 15 Oct 2020 17:59
Operator : CG/JU
Sample : L4408-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WP-1

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-BP101420.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003629.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.010	16	21	28	rVB	53651	61673	1.08%	0.227%
2	3.275	57	66	76	rBV	584436	1035861	18.10%	3.816%
3	3.363	76	81	98	rVB	1534906	1888964	33.01%	6.958%
4	5.499	438	444	450	rBV	121120	170930	2.99%	0.630%
5	6.028	525	534	545	rBV	810853	1192239	20.83%	4.392%
6	7.675	807	814	823	rBV	654600	1058658	18.50%	3.900%
7	8.093	878	885	892	rBV	43081	67797	1.18%	0.250%
8	8.540	954	961	968	rBV	336880	539818	9.43%	1.989%
9	9.704	1151	1159	1170	rBV	934252	1530694	26.75%	5.639%
10	11.386	1436	1445	1458	rBV	416865	709734	12.40%	2.614%
11	12.204	1577	1584	1591	rVB	52232	88888	1.55%	0.327%
12	13.769	1841	1850	1860	rBV	2477814	3518199	61.48%	12.960%
13	14.551	1978	1983	1989	rBV	311124	431936	7.55%	1.591%
14	15.139	2076	2083	2091	rVB	674781	982211	17.16%	3.618%
15	16.604	2326	2332	2343	rBV	1368745	1947012	34.02%	7.172%
16	17.857	2538	2545	2551	rBV	846291	1204332	21.05%	4.436%
17	18.663	2677	2682	2690	rBV	416628	584470	10.21%	2.153%
18	18.727	2691	2693	2705	rVB	36407	70218	1.23%	0.259%
19	19.857	2881	2885	2901	rBV	142605	208724	3.65%	0.769%
20	20.321	2958	2964	2969	rBV	4727872	5722323	100.00%	21.079%
21	21.486	3158	3162	3172	rBV	950101	1047220	18.30%	3.858%
22	21.862	3220	3226	3232	rBV	984947	1328542	23.22%	4.894%
23	21.951	3237	3241	3249	rVB5	41505	78691	1.38%	0.290%
24	22.445	3319	3325	3331	rBV5	60071	108697	1.90%	0.400%
25	24.439	3656	3664	3673	rVB2	629454	1298856	22.70%	4.785%
26	25.050	3762	3768	3778	rBV2	120275	270040	4.72%	0.995%

Sum of corrected areas: 27146727

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Instrument :
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ClientSampleId :
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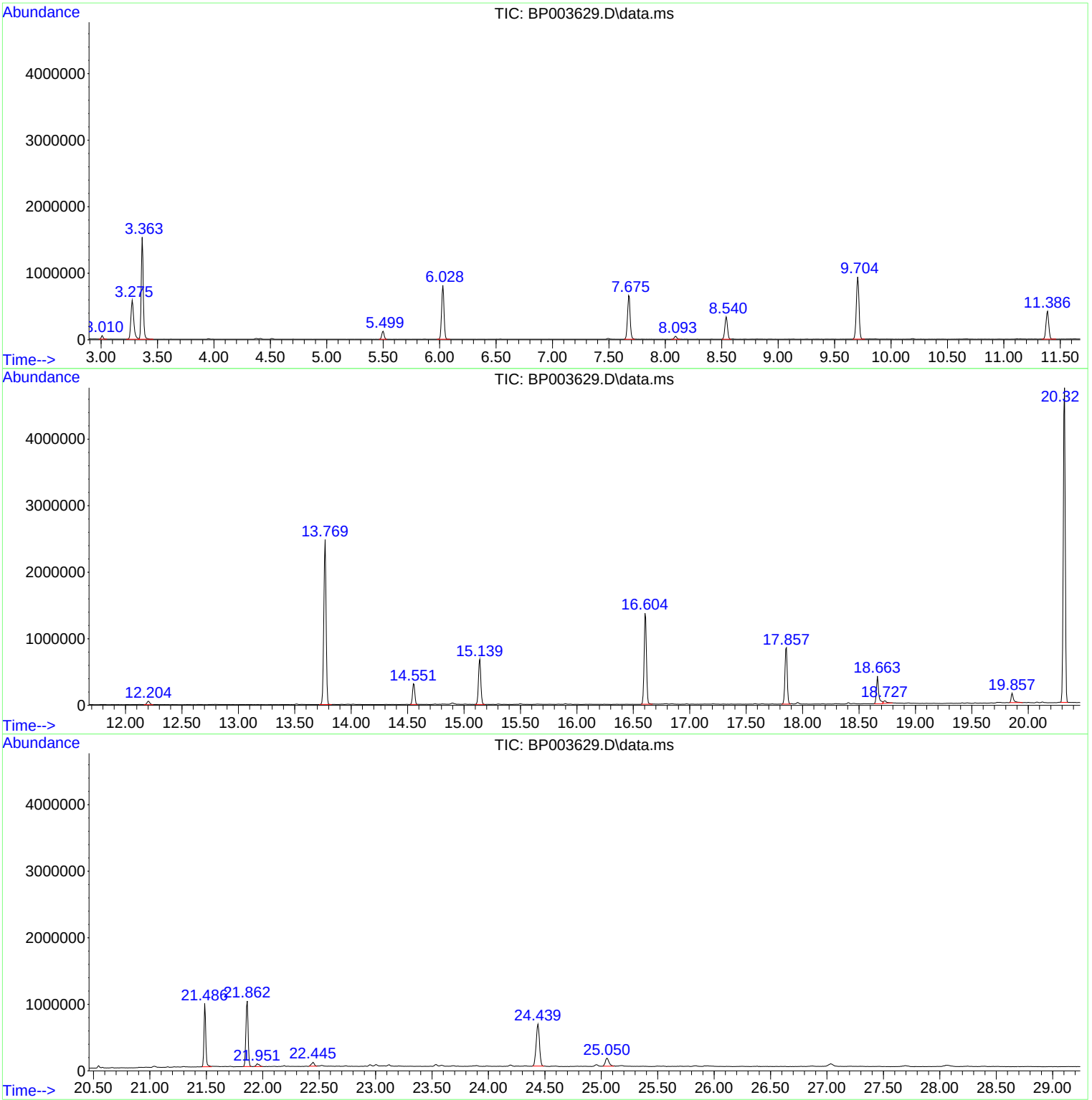
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

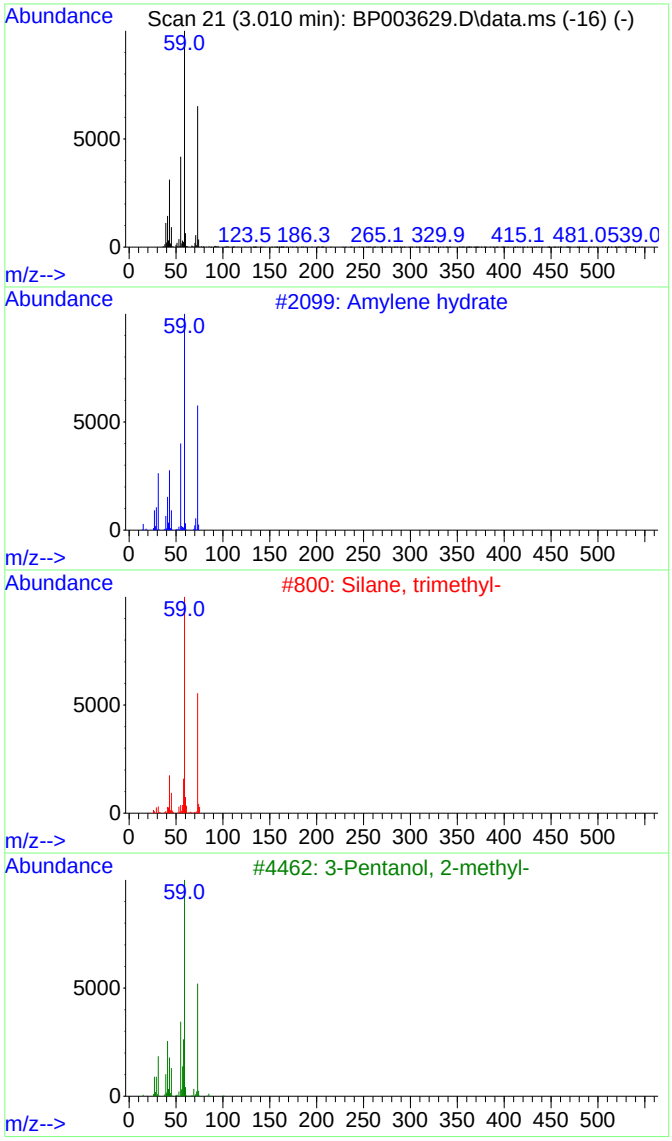
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

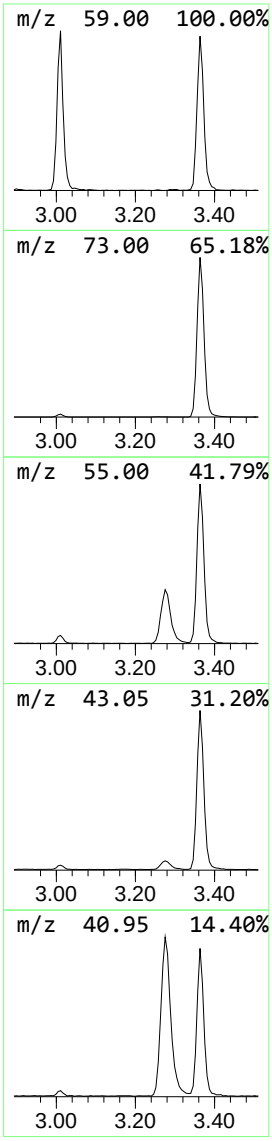
****

Peak Number 1 Amylene hydrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.010	2.28 ng	61673	1,4-Dichlorobenzene-d4	8.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	78
2	Silane, trimethyl-	74	C3H10Si	000993-07-7	72
3	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	64
4	4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	40
5	2-Hexanone, 3-hydroxy-3,5-dimethyl-	144	C8H16O2	006321-14-8	36





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Sample : L4408-10
Misc :
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Instrument :
BNA_P
ClientSampleId :
WP-1

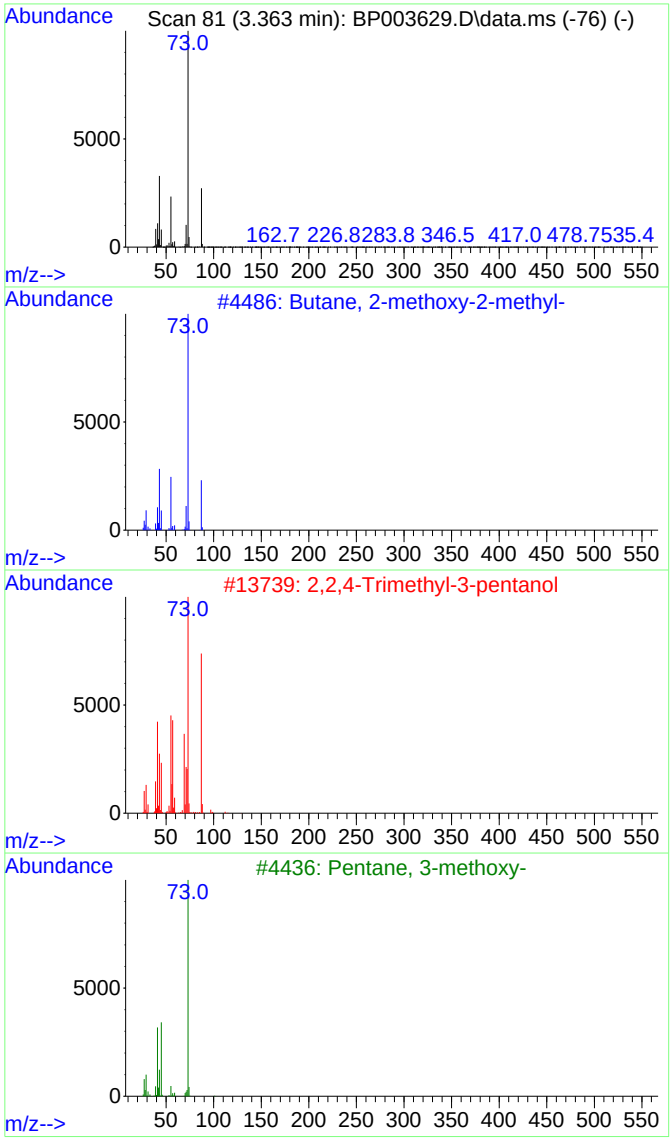
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

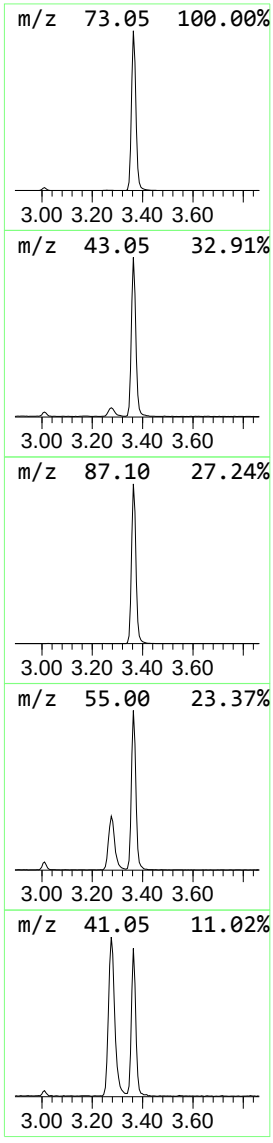
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	69.99 ng	1888960	1,4-Dichlorobenzene-d4	8.540

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	56
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Operator : CG/JU
Sample : L4408-10
Misc :
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Instrument : BNA_P
ClientSampleId : WP-1

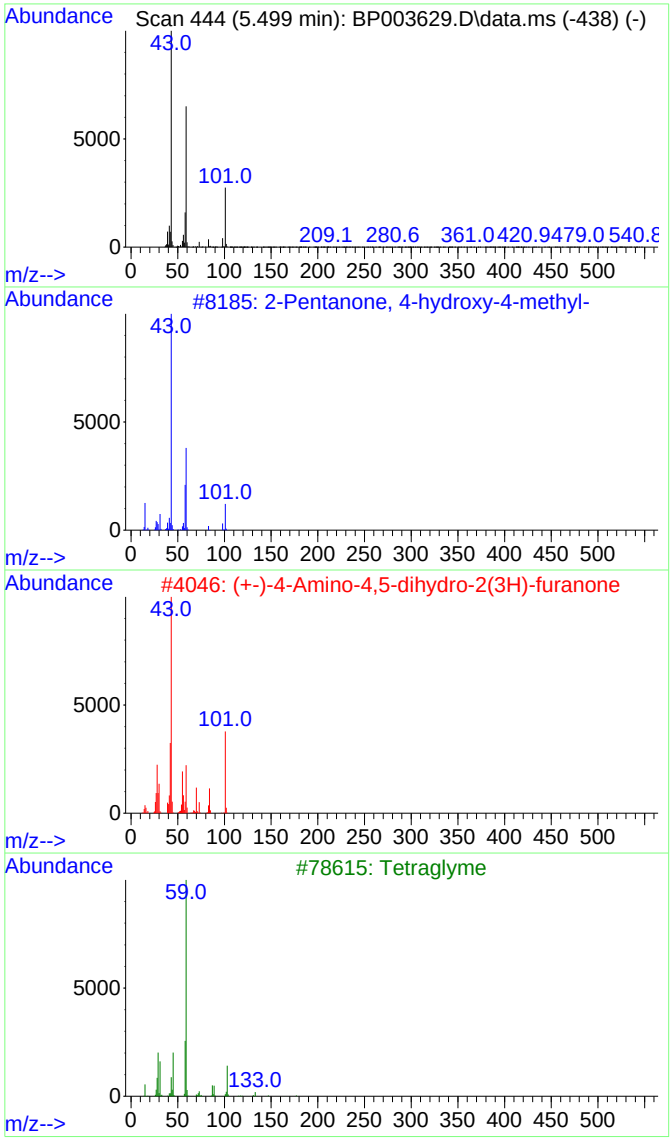
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

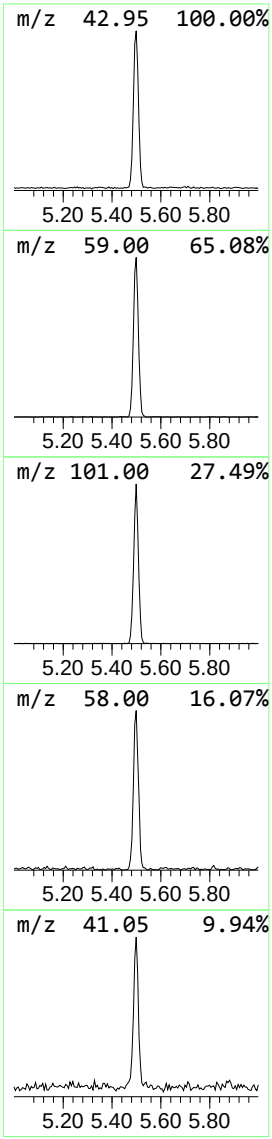
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.499	6.33 ng	170930	1,4-Dichlorobenzene-d4	8.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
3	Tetraglyme	222	C10H22O5	000143-24-8	25
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23
5	Acetone	58	C3H6O	000067-64-1	9





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Operator : CG/JU
Sample : L4408-10
Misc :
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Instrument : BNA_P
ClientSampleId : WP-1

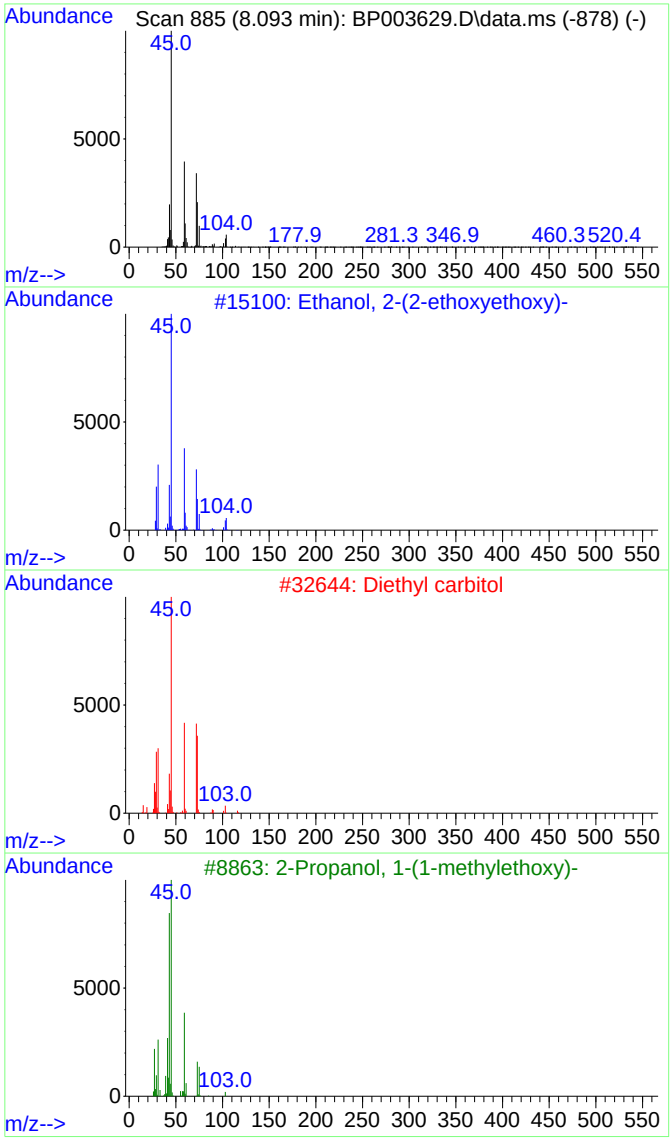
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

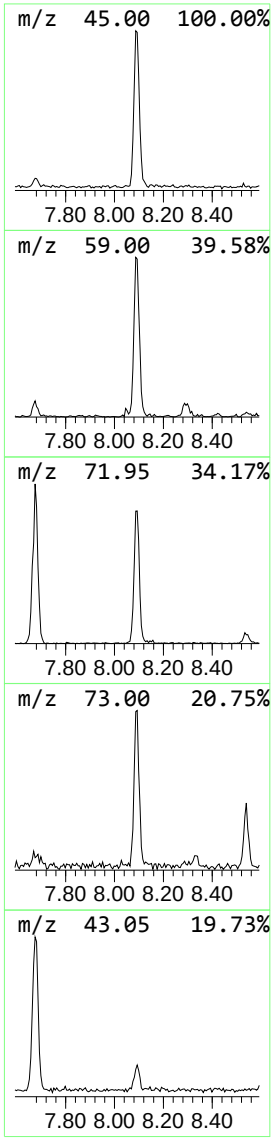
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.093	2.51 ng	67797	1,4-Dichlorobenzene-d4	8.540

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	64
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	42





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Operator : CG/JU
Sample : L4408-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : WP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

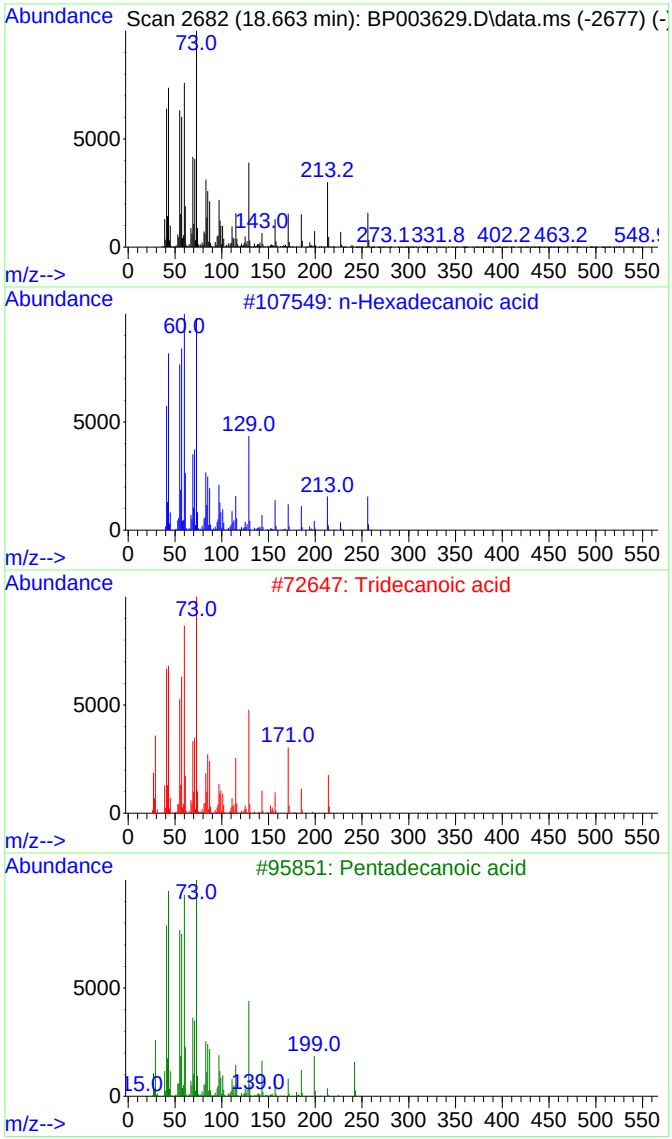
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

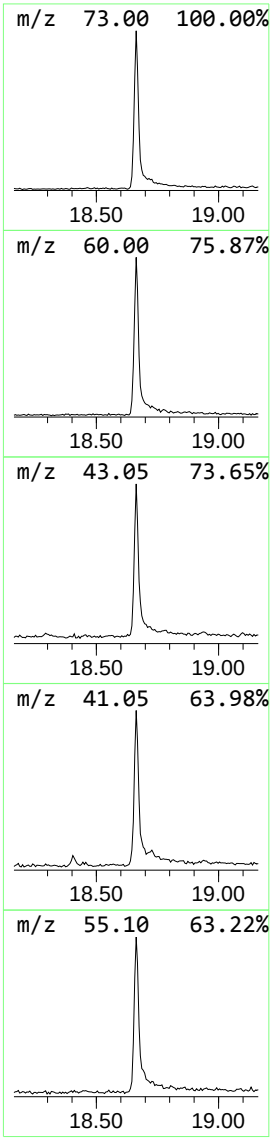
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.663	9.71 ng	584470	Phenanthrene-d10	17.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Instrument : BNA_P
ClientSampleId : WP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP101420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

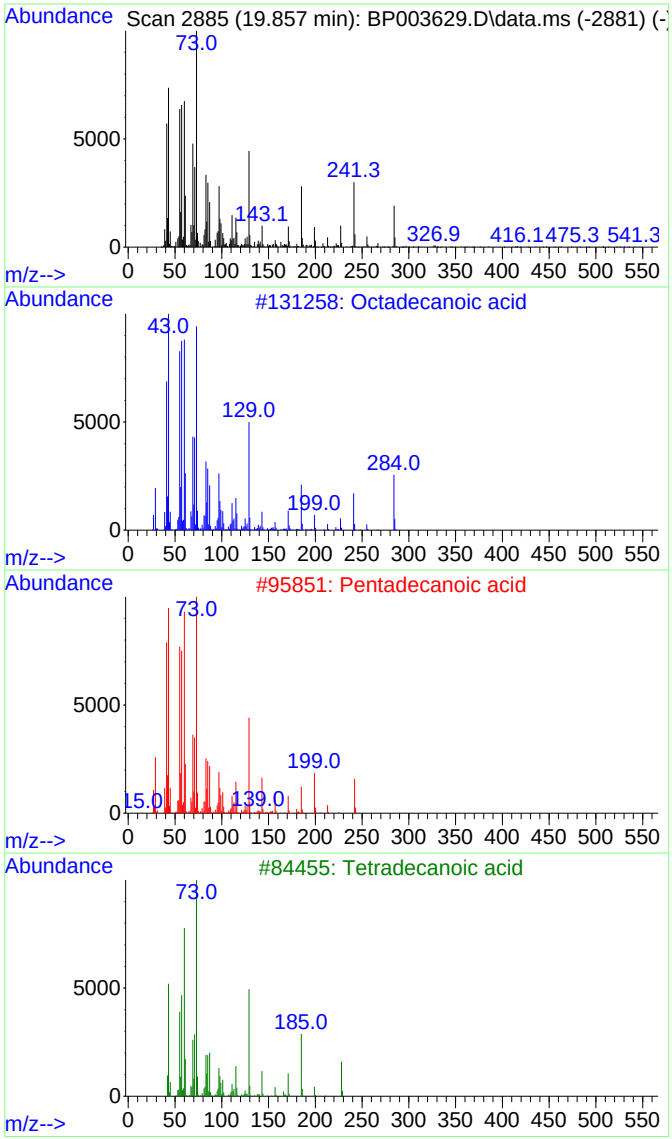
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

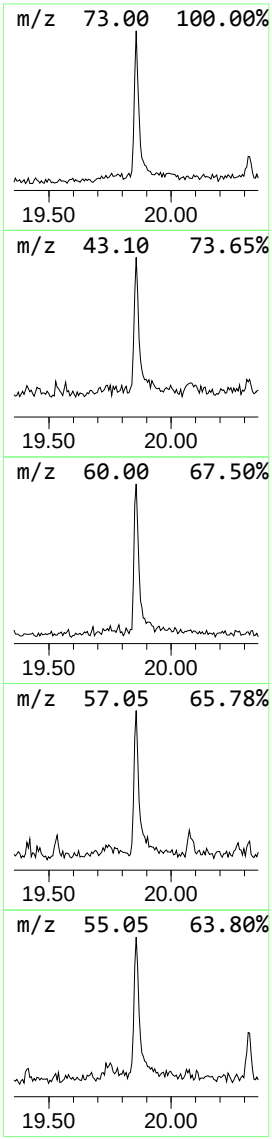
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.857	3.47 ng	208724	Phenanthrene-d10	17.857

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	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25





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Instrument : BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

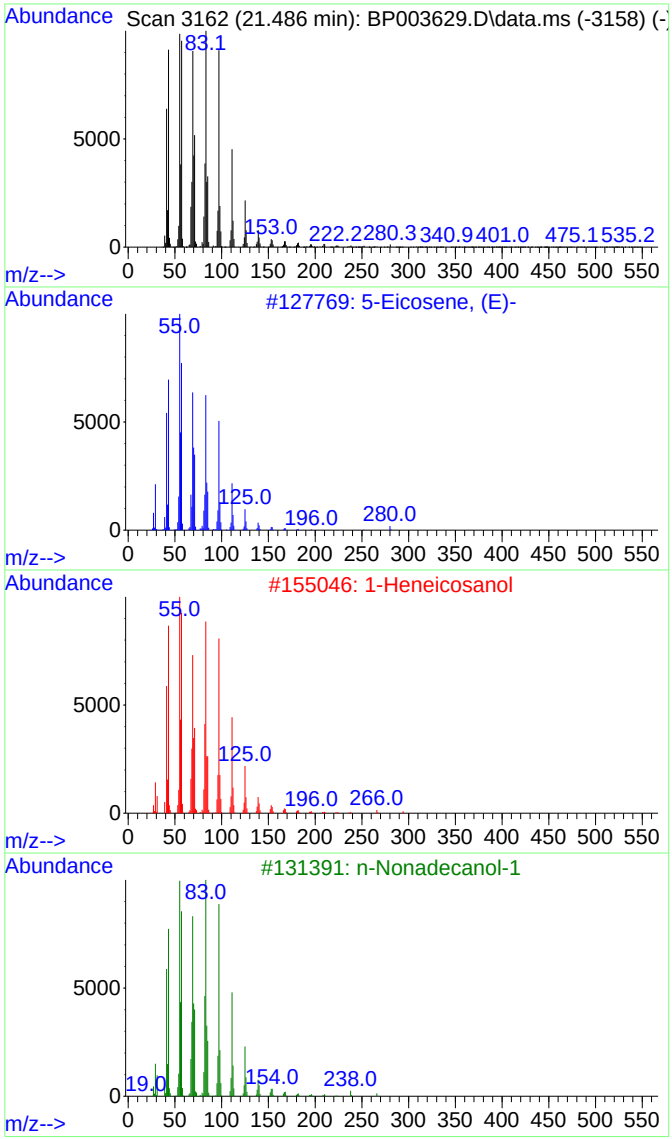
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

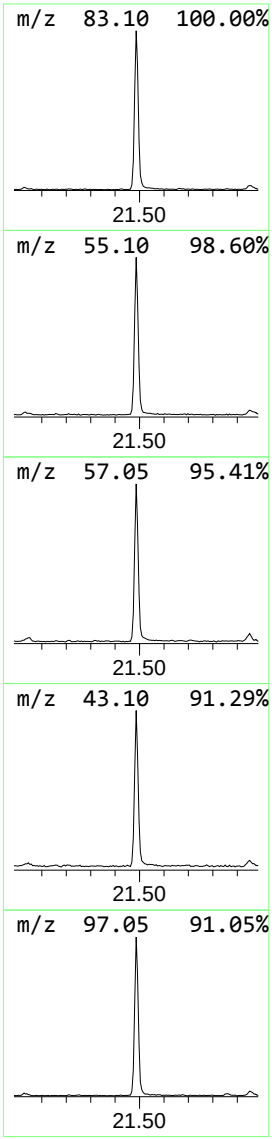
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.486	15.77 ng	1047220	Chrysene-d12	21.862

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93





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TIC Library : C:\DATABASE\NIST11.L
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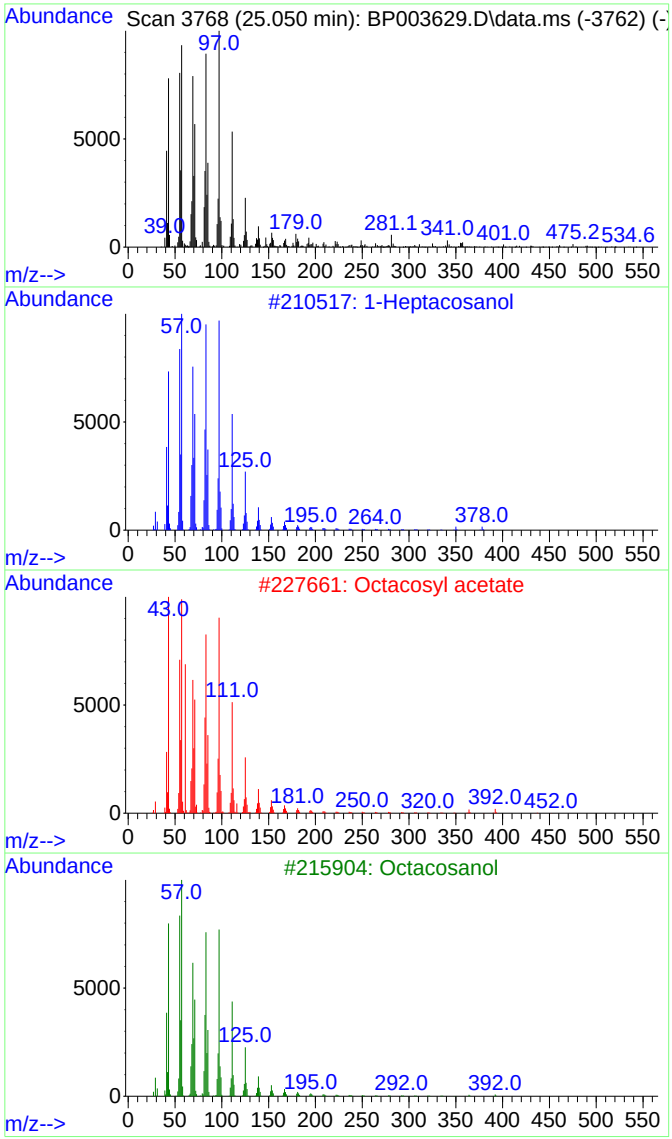
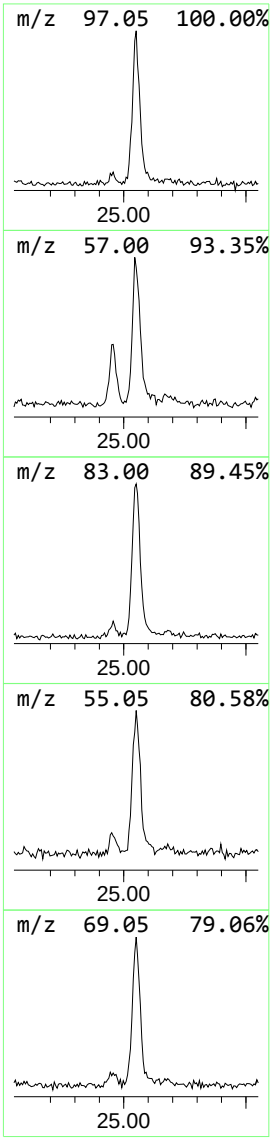
****

Peak Number 9 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.051	4.16 ng	270040	Perylene-d12	24.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Octacosyl acetate	452	C30H60O2	018206-97-8	93
3	Octacosanol	410	C28H58O	000557-61-9	93
4	17-Pentatriacontene	491	C35H70	006971-40-0	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





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
Amylene hydrate	3.010	2.3	ng	61673	1	8.540	539818	20.0
Butane, 2-metho...	3.363	70.0	ng	1888960	1	8.540	539818	20.0
2-Pentanone, 4-...	5.499	6.3	ng	170930	1	8.540	539818	20.0
Ethanol, 2-(2-e...	8.093	2.5	ng	67797	1	8.540	539818	20.0
n-Hexadecanoic ...	18.663	9.7	ng	584470	4	17.857	1204330	20.0
Octadecanoic acid	19.857	3.5	ng	208724	4	17.857	1204330	20.0
5-Eicosene, (E)-	21.486	15.8	ng	1047220	5	21.862	1328540	20.0
1-Heptacosanol	25.051	4.2	ng	270040	6	24.439	1298860	20.0