LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021822\
Data File : BP009218.D
Acq On : 18 Feb 2022 17:35
Operator : CG/JU
Sample : N1573-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : MW-25R

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\8270E-BP020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009218.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.963	161	166	179	rVB	132318	233711	1.26%	0.388%
2	4.251	210	215	231	rVB	183867	324960	1.75%	0.540%
3	4.893	318	324	345	rVB	139388	280051	1.51%	0.465%
4	5.363	398	404	409	rBV	1127737	2014104	10.86%	3.345%
5	5.775	467	474	489	rVB	189421	337164	1.82%	0.560%
6	6.969	671	677	698	rBV	582956	1447264	7.81%	2.404%
7	7.569	772	779	792	rBV	108541	248912	1.34%	0.413%
8	7.763	805	812	820	rBV	482688	848014	4.57%	1.409%
9	8.928	1003	1010	1041	rBV	1627299	3407974	18.38%	5.660%
10	10.563	1281	1288	1295	rBV	580680	1184677	6.39%	1.968%
11	12.763	1656	1662	1678	rBV	176792	317504	1.71%	0.527%
12	13.028	1699	1707	1735	rBV	6335510	10144076	54.71%	16.849%
13	13.263	1741	1747	1767	rVB	641452	1118959	6.03%	1.859%
14	14.410	1935	1942	1950	rBV	1161690	1908060	10.29%	3.169%
15	15.239	2076	2083	2092	rVB	169705	249894	1.35%	0.415%
16	15.786	2171	2176	2184	rBV	125746	194195	1.05%	0.323%
17	15.916	2191	2198	2216	rBV	4384408	7741782	41.75%	12.859%
18	17.174	2406	2412	2427	rBV	1556434	2500740	13.49%	4.154%
19	17.839	2520	2525	2531	rBV	167456	220317	1.19%	0.366%
20	19.739	2842	2848	2863	rBV	14378369	18542374	100.00%	30.798%
21	21.280	3104	3110	3124	rBV	2192903	3490886	18.83%	5.798%
22	23.662	3508	3515	3532	rVB2	1540561	3450835	18.61%	5.732%

Sum of corrected areas: 60206453

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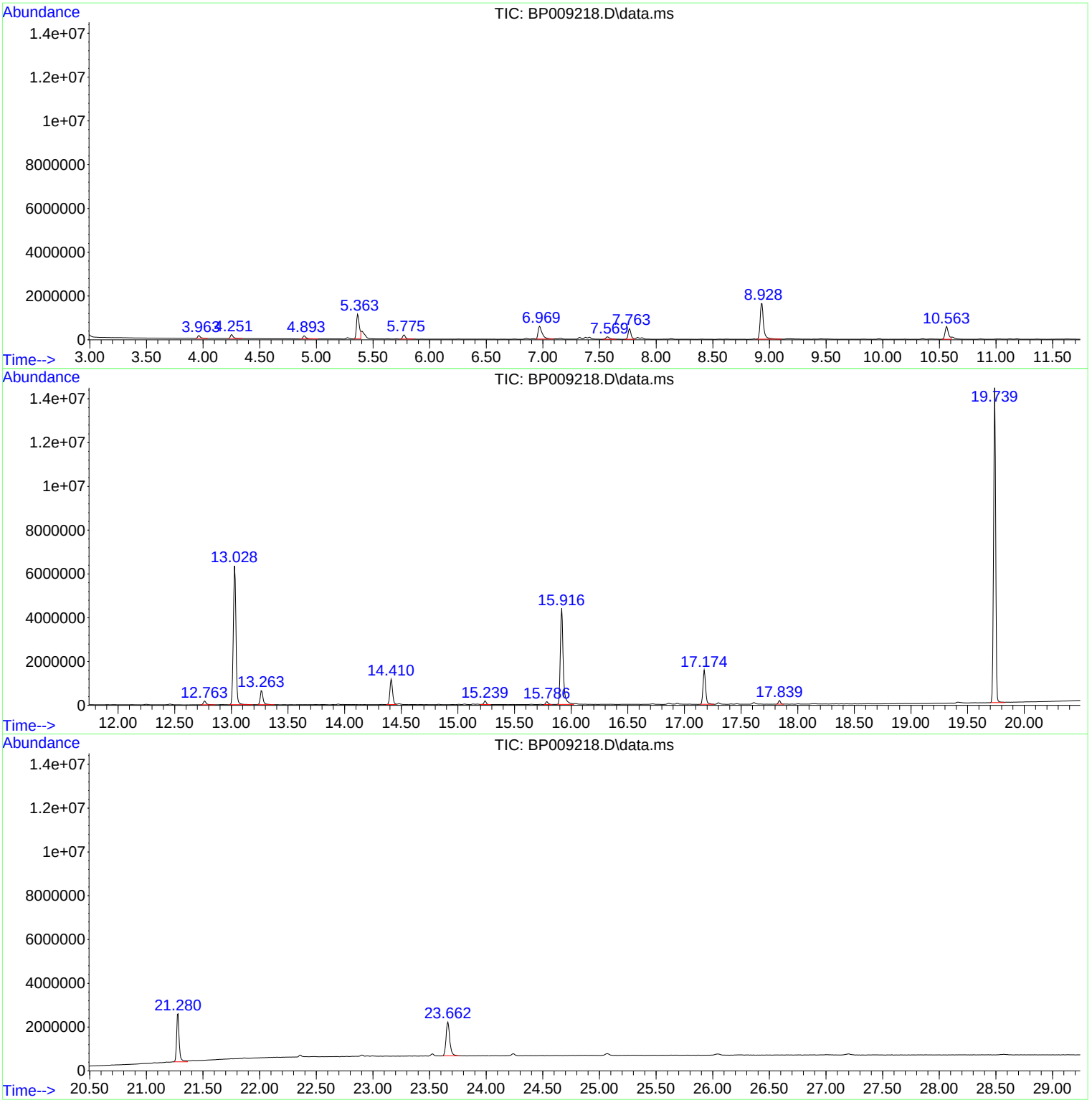
Instrument :
BNA_P
ClientSampleId :
MW-25R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.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 : BP009218.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

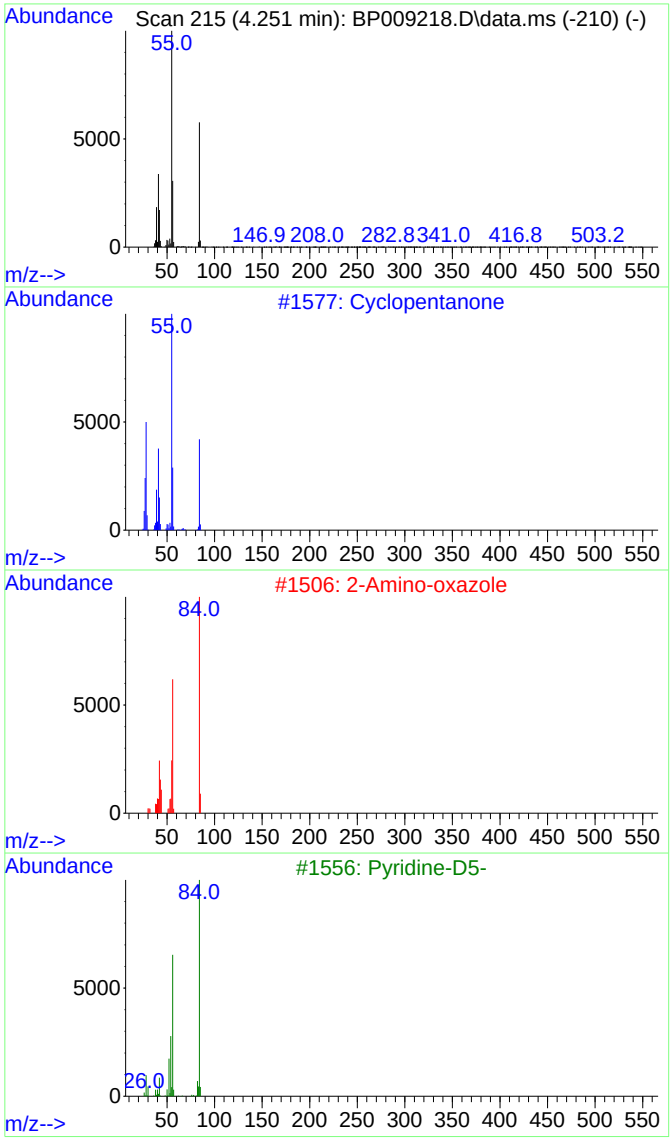
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

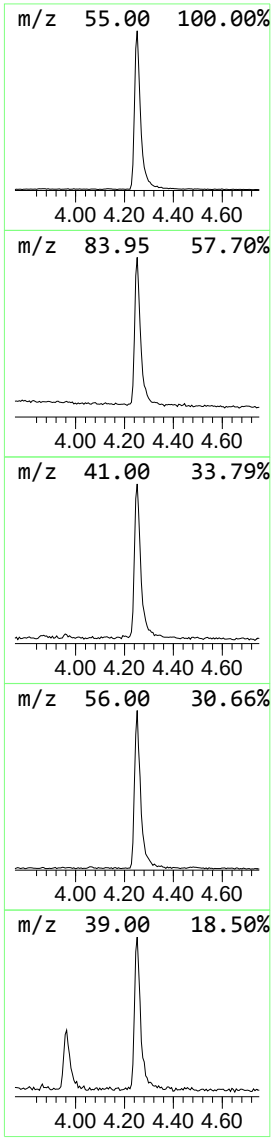
****

Peak Number 2 Cyclopentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.251	7.66 ng	324960	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	91
2	2-Amino-oxazole	84	C3H4N2O	004570-45-0	53
3	Pyridine-D5-	84	C5D5N	007291-22-7	52
4	2(5H)-Furanone	84	C4H4O2	000497-23-4	52
5	3-Aminoisoxazole	84	C3H4N2O	001750-42-1	50





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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-25R

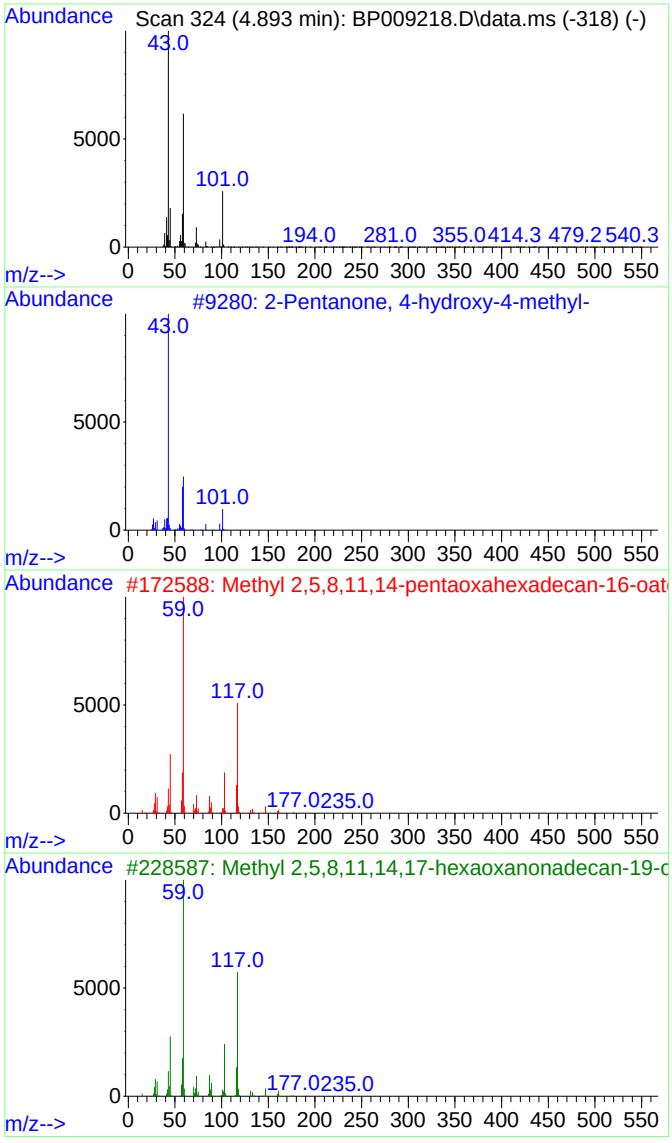
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

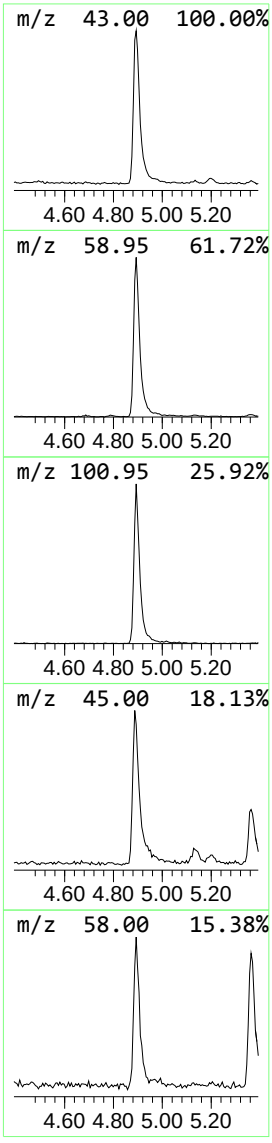
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	6.60 ng	280051	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Methyl 2,5,8,11,14-pentaoxahexad...	280	C12H24O7	1000366-81-5	38
3	Methyl 2,5,8,11,14,17-hexaoxanon...	324	C14H28O8	1000366-81-4	38
4	Carbonic acid, 2-methoxyethyl 3,...	232	C10H10F2O4	1000357-86-6	37
5	Tetraglyme	222	C10H22O5	000143-24-8	37





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Operator : CG/JU
Sample : N1573-10
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-25R

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

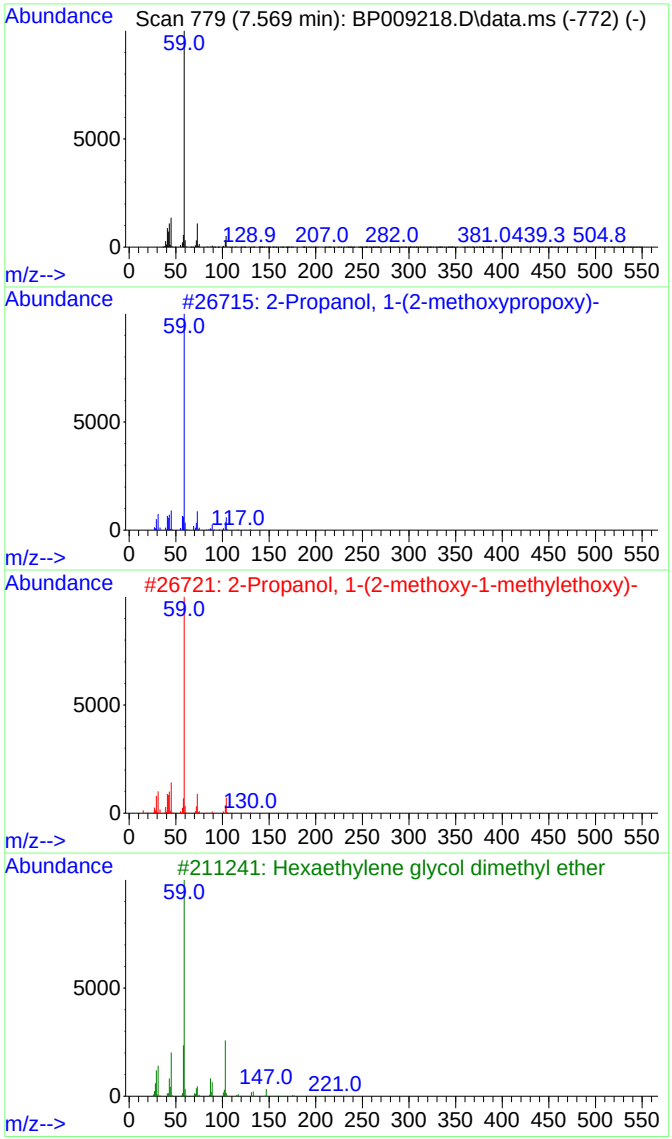
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

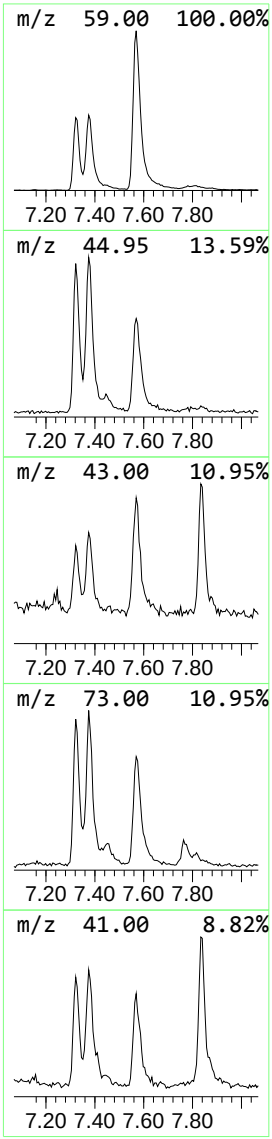
****

Peak Number 5 2-Propanol, 1-(2-methoxypro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.569	5.87 ng	248912	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
3	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	50
4	1-(1-Methoxypropan-2-yloxy)propa...	190	C9H18O4	1000367-08-6	40
5	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	40





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ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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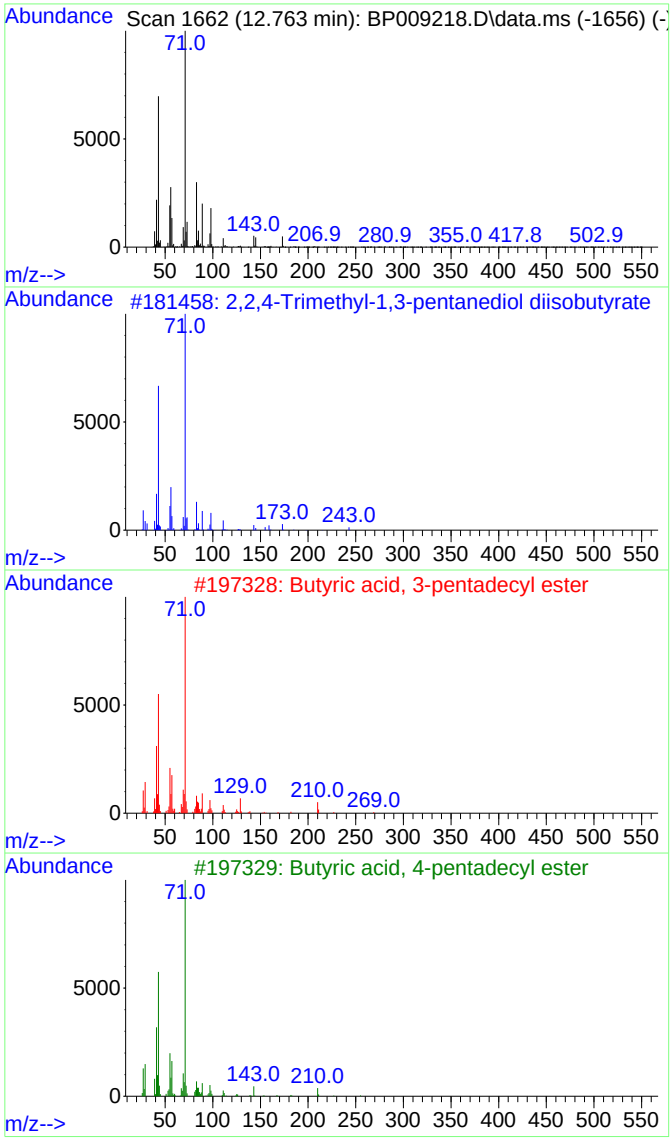
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

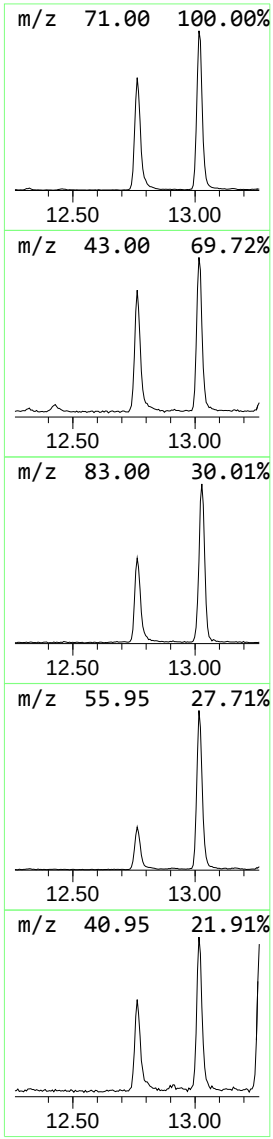
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.763	3.33 ng	317504	Acenaphthene-d10	14.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2	Butyric acid, 3-pentadecyl ester	298	C19H38O2	1000280-57-3	43
3	Butyric acid, 4-pentadecyl ester	298	C19H38O2	1000280-57-4	43
4	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42
5	Sulfurous acid, bis(2-pentyl) ester	222	C10H22O3S	1000309-15-3	38





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Sample : N1573-10
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Instrument :
BNA_P
ClientSampleId :
MW-25R

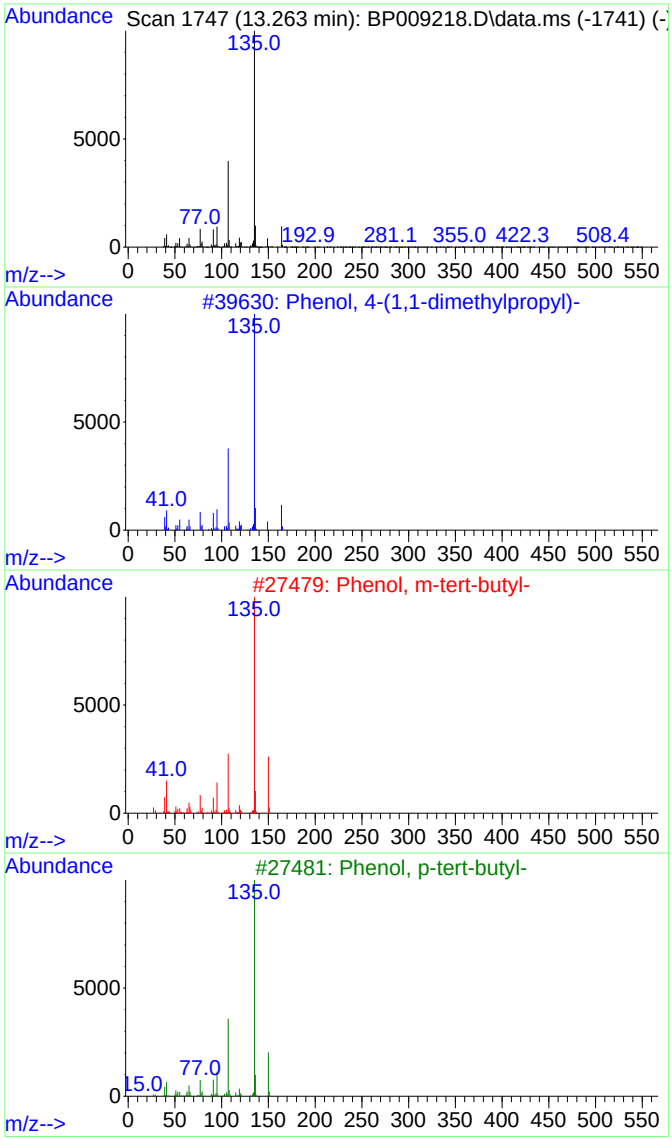
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

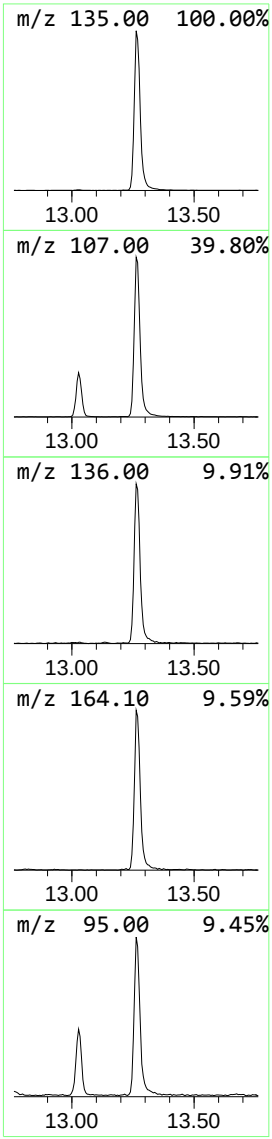
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.263	11.73 ng	1118960	Acenaphthene-d10	14.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	86
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	80
4	Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	64
5	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64





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Misc :
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Instrument :
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ClientSampleId :
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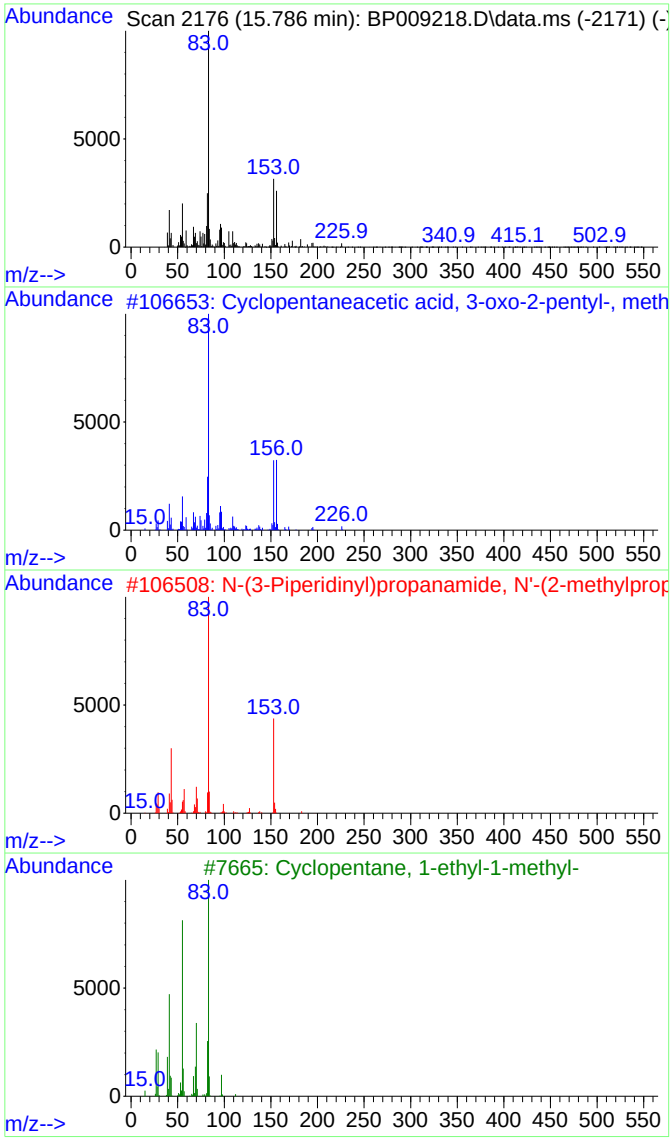
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

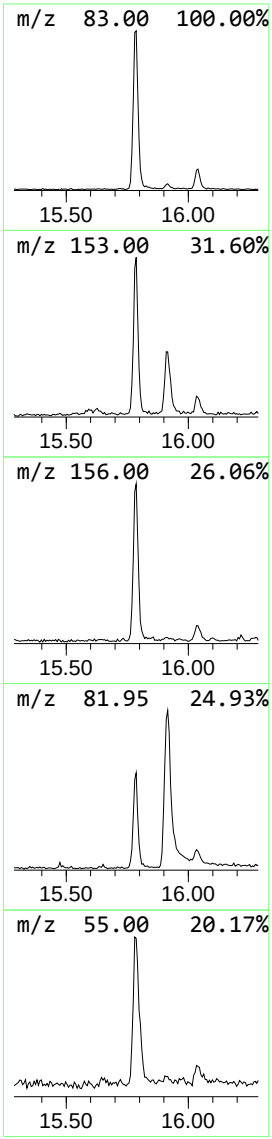
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopentaneacetic acid, 3-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	2.04 ng	194195	Acenaphthene-d10	14.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	98
2	N-(3-Piperidinyl)propanamide, N'...	226	C12H22N2O2	1000469-85-0	47
3	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	47
4	Isocitronellol	156	C10H20O	018479-52-2	47
5	1,5-Pentanediol, O,O'-di(3-methy...	268	C15H24O4	1010331-15-6	43





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
Cyclopentanone	4.251	7.7	ng	324960	1	7.763	848014	20.0
2-Pentanone, 4-...	4.893	6.6	ng	280051	1	7.763	848014	20.0
2-Propanol, 1-(...	7.569	5.9	ng	248912	1	7.763	848014	20.0
2,2,4-Trimethyl...	12.763	3.3	ng	317504	3	14.410	1908060	20.0
Phenol, 4-(1,1-...	13.263	11.7	ng	1118960	3	14.410	1908060	20.0
Cyclopentaneace...	15.786	2.0	ng	194195	3	14.410	1908060	20.0