LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005881.D
Acq On : 11 Jun 2021 20:55
Operator : CG/JU
Sample : M2625-20
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(214-218)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005881.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.440	225	230	239	rVB	24891	37722	1.09%	0.284%
2	5.046	328	333	343	rVB	31760	44492	1.29%	0.335%
3	5.511	406	412	432	rBV	473178	755278	21.86%	5.683%
4	7.111	676	684	699	rBV	561964	969327	28.05%	7.294%
5	7.246	701	707	726	rVB	44804	113126	3.27%	0.851%
6	7.946	819	826	834	rBV	230821	368758	10.67%	2.775%
7	8.605	932	938	950	rBV	64542	136697	3.96%	1.029%
8	9.110	1016	1024	1034	rBV	398432	679814	19.67%	5.115%
9	10.546	1262	1268	1281	rBV3	27019	75387	2.18%	0.567%
10	10.752	1294	1303	1313	rBV	263942	468306	13.55%	3.524%
11	12.028	1512	1520	1532	rBV3	29844	67342	1.95%	0.507%
12	13.040	1685	1692	1705	rBV2	20637	60564	1.75%	0.456%
13	13.199	1712	1719	1743	rBV	1408282	2121164	61.39%	15.961%
14	13.998	1850	1855	1861	rBV	24228	38075	1.10%	0.287%
15	14.569	1944	1952	1970	rBV	364906	604965	17.51%	4.552%
16	16.063	2200	2206	2217	rBV	77493	147169	4.26%	1.107%
17	17.316	2411	2419	2433	rBV	449515	745897	21.59%	5.613%
18	19.863	2846	2852	2862	rBV	2713630	3455377	100.00%	26.001%
19	21.092	3057	3061	3069	rBV4	55807	115290	3.34%	0.868%
20	21.386	3106	3111	3120	rBV	811393	1057716	30.61%	7.959%
21	23.804	3515	3522	3538	rVB2	572287	1227162	35.51%	9.234%

Sum of corrected areas: 13289628

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005881.D
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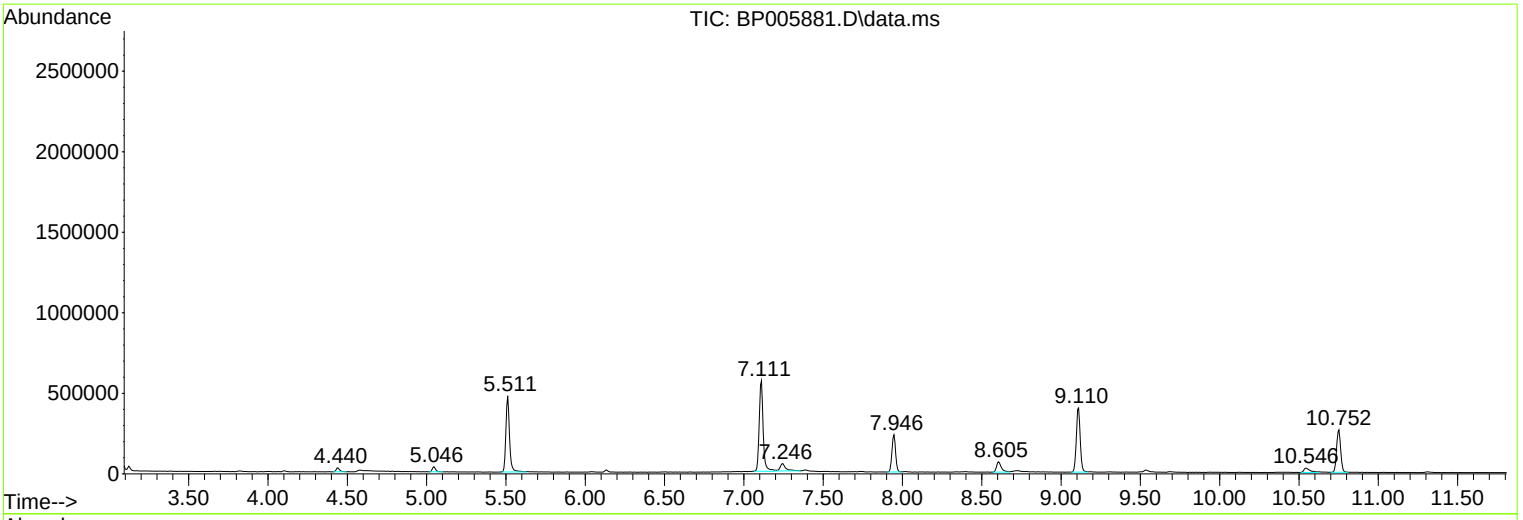
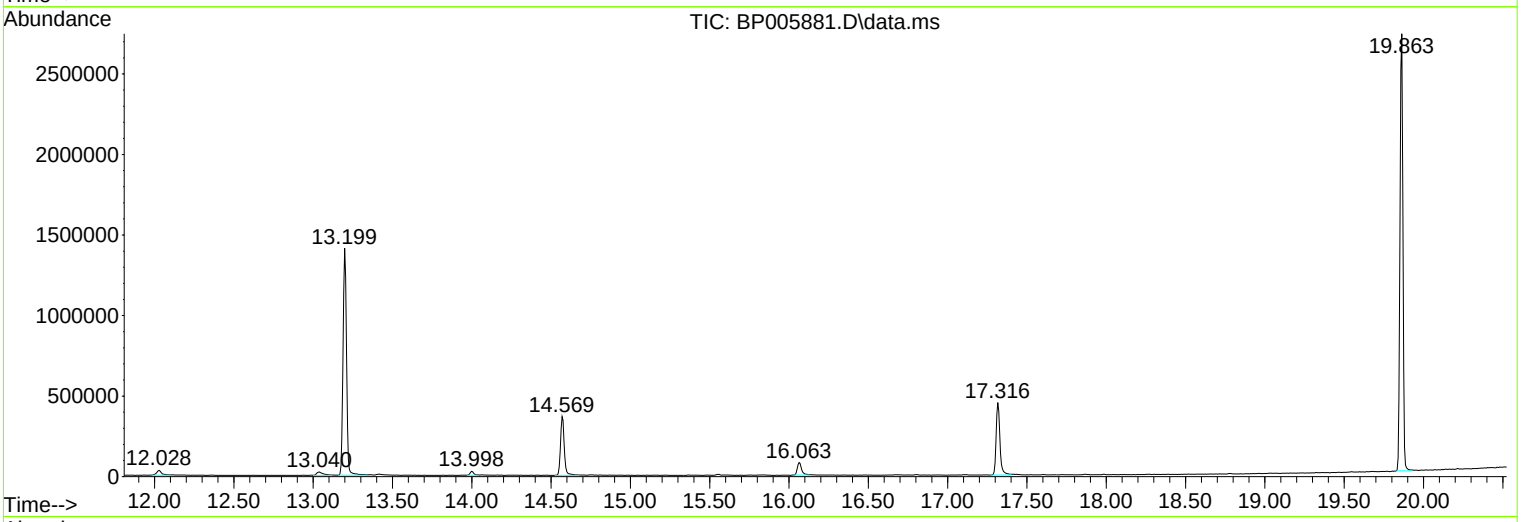
Sample : M2625-20
Misc :
ALS Vial : 18 Sample Multiplier: 1

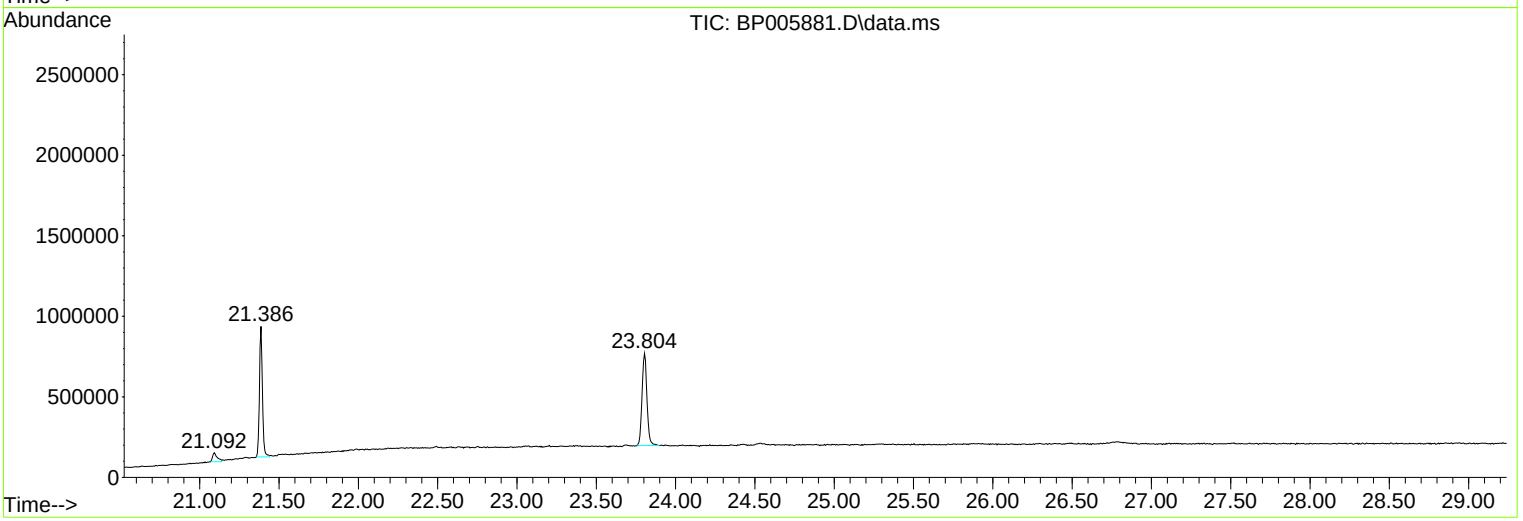
Instrument :
BNA_P
ClientSampleId :
18-B12(214-218)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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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Data File : BP005881.D
Acq On : 11 Jun 2021 20:55
Operator : CG/JU
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Instrument :
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ClientSampleId :
18-B12(214-218)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

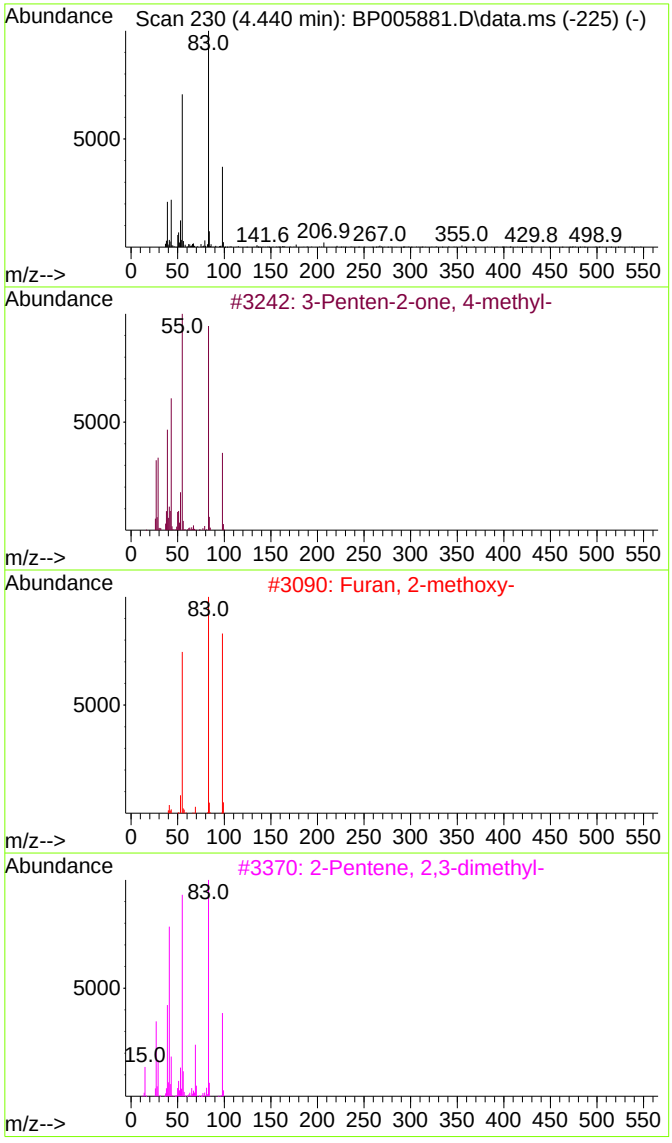
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

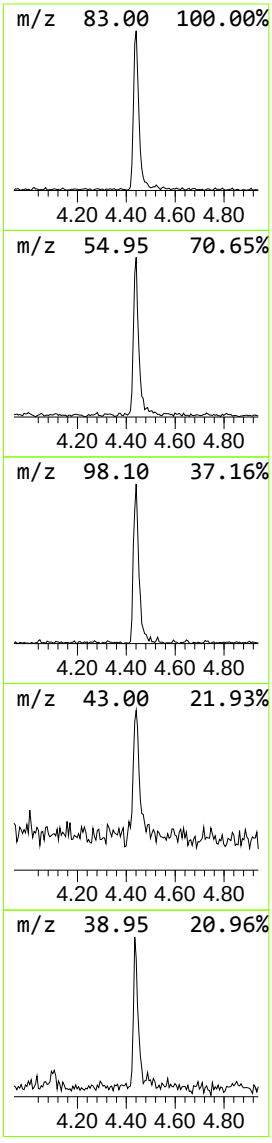
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.440	2.05 ng	37722	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	87
2	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	86
3	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86
4	3-Hexen-2-one	98	C6H10O	000763-93-9	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86





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Data File : BP005881.D
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Operator : CG/JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
18-B12(214-218)

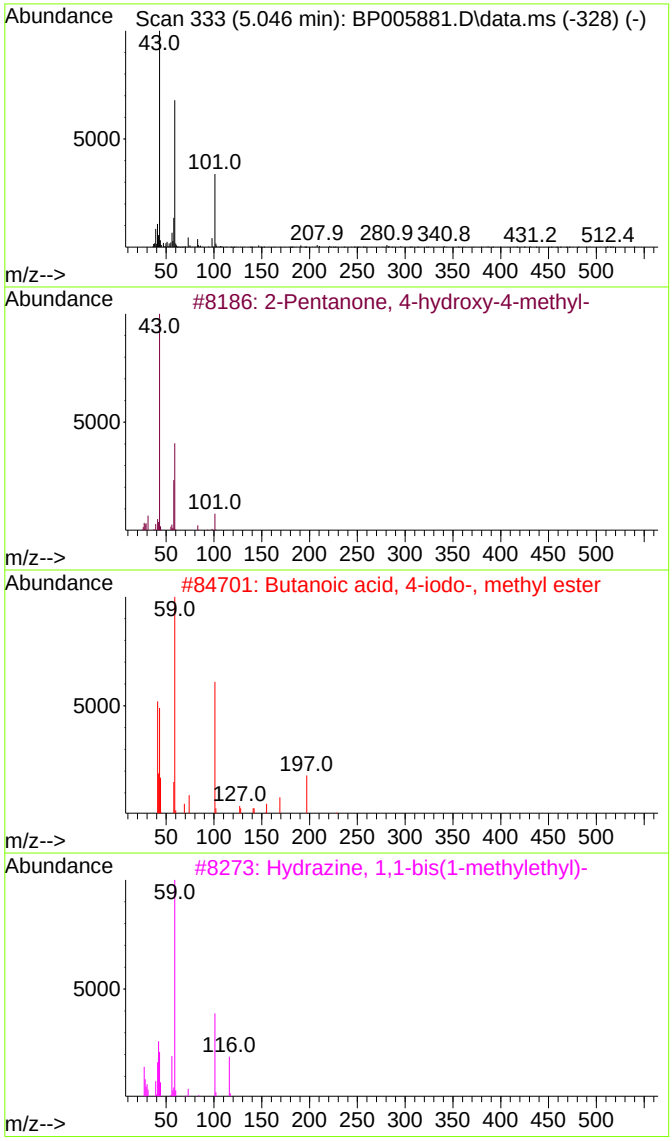
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

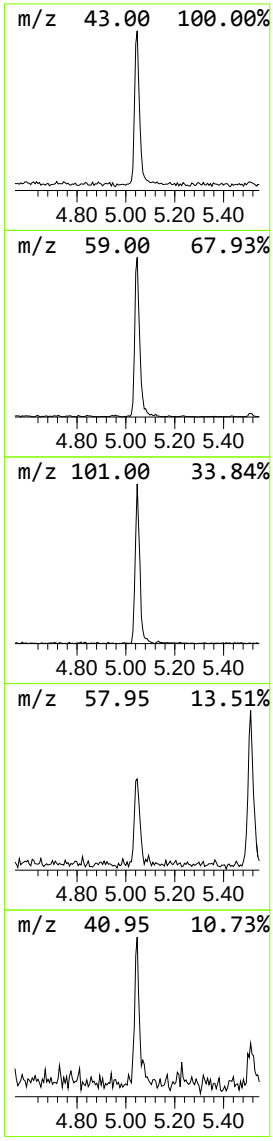
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	2.41 ng	44492	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	33
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005881.D
Acq On : 11 Jun 2021 20:55
Operator : CG/JU
Sample : M2625-20
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B12(214-218)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

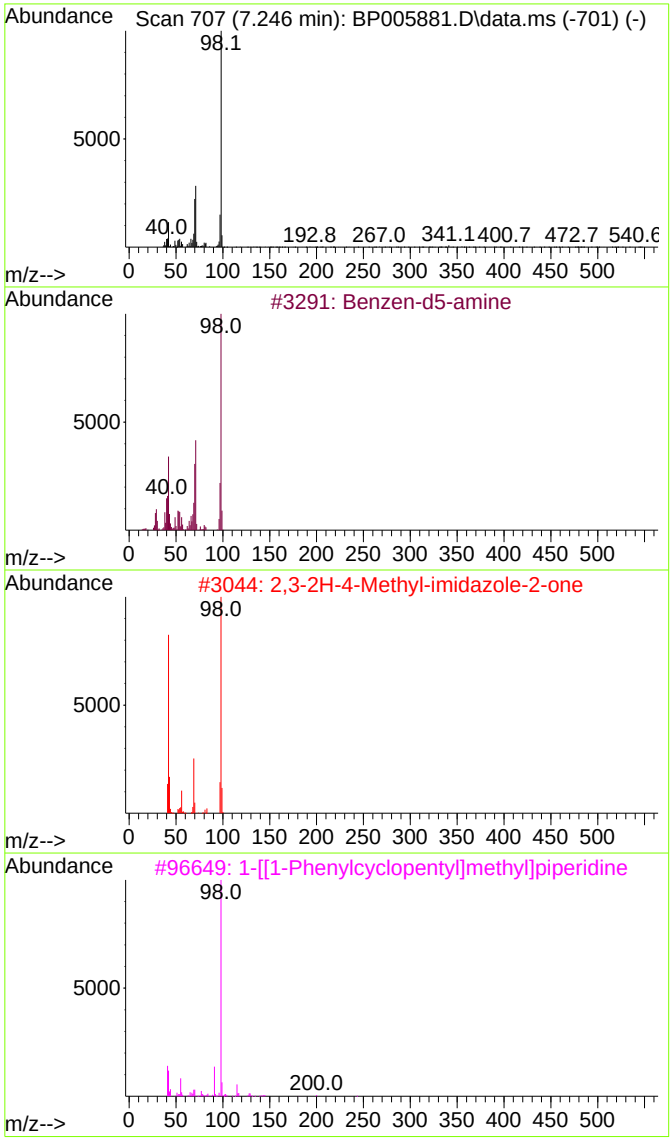
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

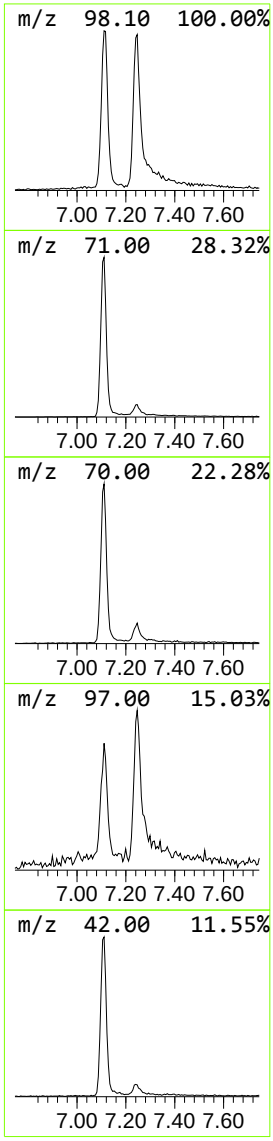
****

Peak Number 3 Benzen-d5-amine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.246	6.14 ng	113126	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	56
2	2,3-2H-4-Methyl-imidazole-2-one	98	C4H6N2O	039799-77-4	47
3	1-[[1-Phenylcyclopentyl]methyl]p...	243	C17H25N	1000214-74-2	47
4	Benzo[b]thiophen-2-carbonitrile,...	303	C16H21N3OS	1000260-31-3	47
5	1-Methyl-2-piperidinemethanol	129	C7H15NO	020845-34-5	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005881.D
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Operator : CG/JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B12(214-218)

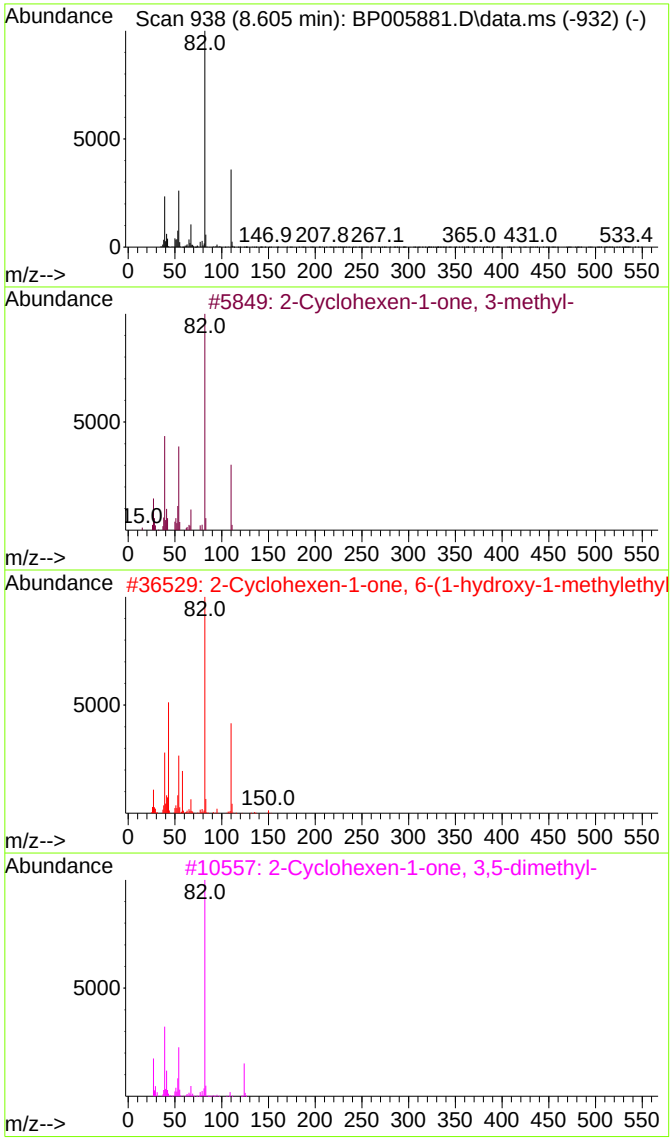
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

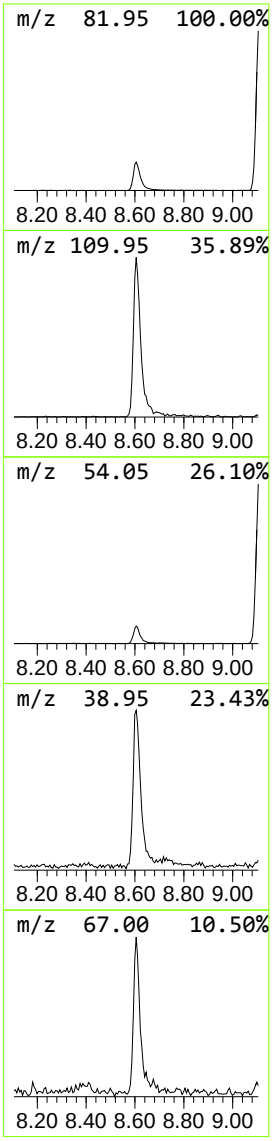
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.605	7.41 ng	136697	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	90
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	64
3	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	64
4	1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	59
5	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	53





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Operator : CG/JU
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B12(214-218)

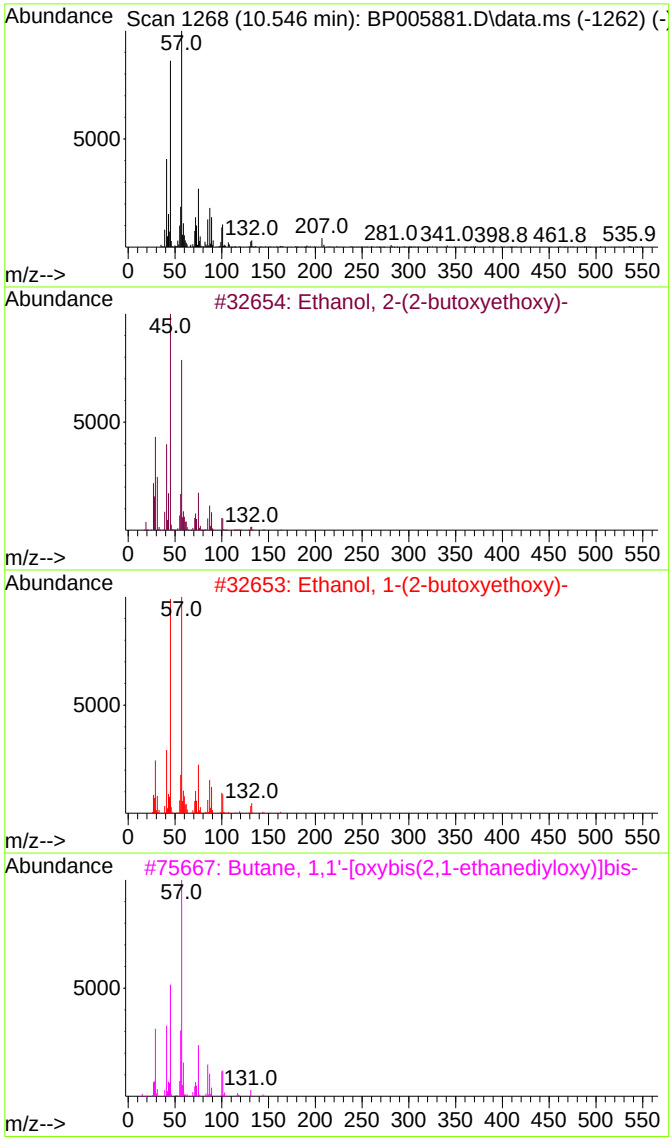
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

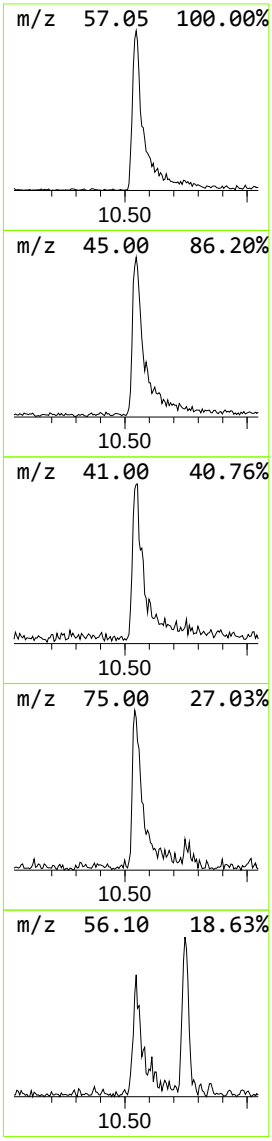
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.546	3.22 ng	75387	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(214-218)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

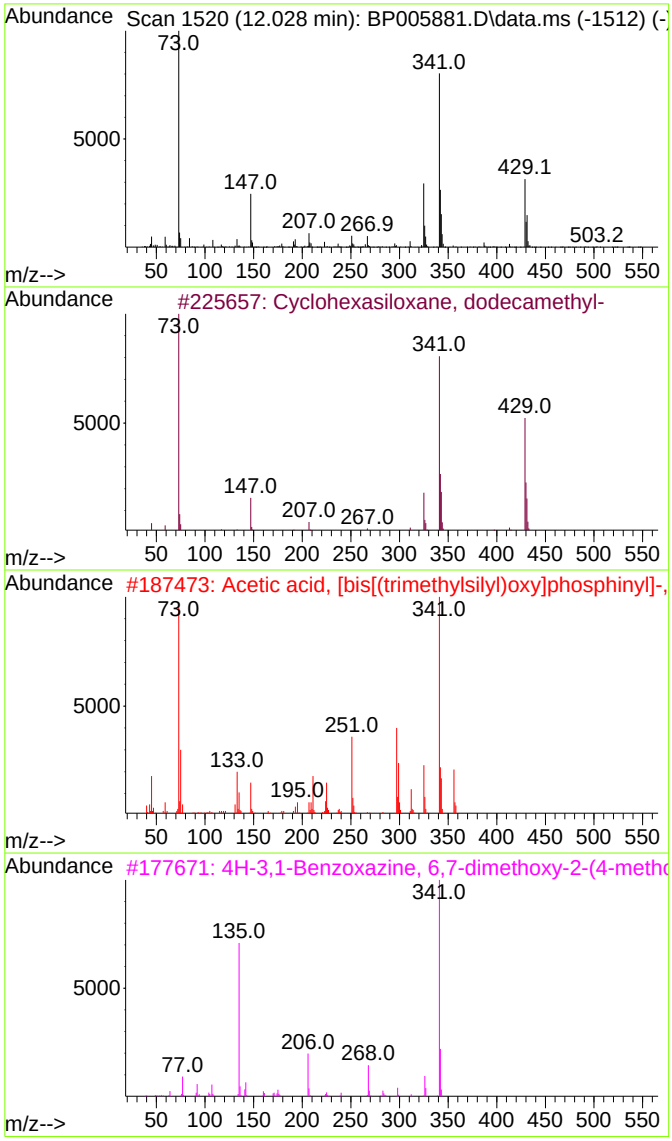
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

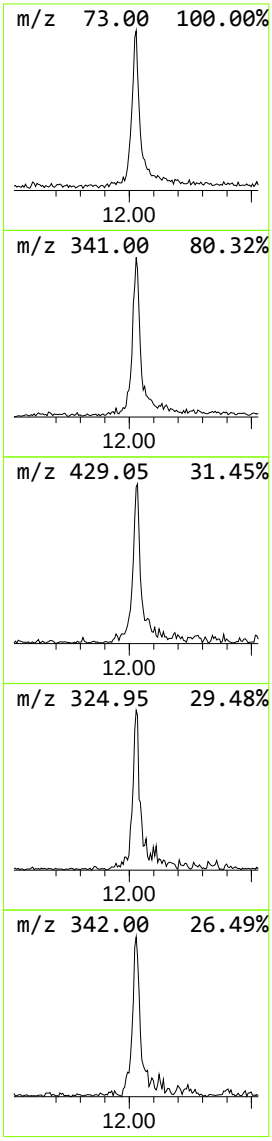
****

Peak Number 6 Cyclohexasiloxane, dodecame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	2.88 ng	67342	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	90
2	Acetic acid, [bis[(trimethylsily...	356	C11H29O5PSi3	053044-27-2	42
3	4H-3,1-Benzoxazine, 6,7-dimethox...	341	C20H23NO4	1000327-27-7	38
4	Isoindole-1,3(1H,3H)-dione, 5-be...	341	C22H15NO3	331269-95-5	27
5	Cobalt, .eta.-5-cyclopentadienyl...	341	C22H18Co	1000161-22-8	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

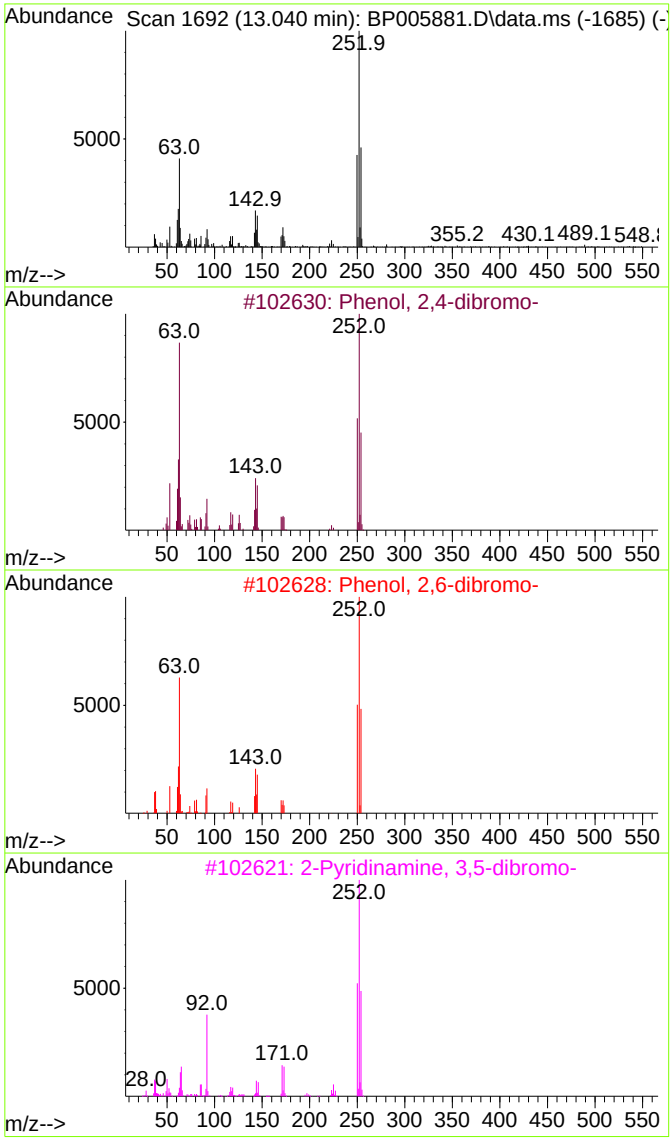
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

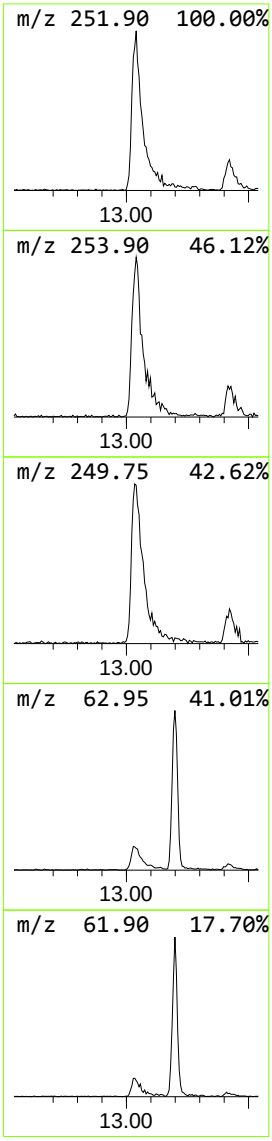
****

Peak Number 7 Phenol, 2,4-dibromo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.040	2.00 ng	60564	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	99
2	Phenol, 2,6-dibromo-	250	C6H4Br2O	000608-33-3	98
3	2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	50
4	Phenol, 2,4-dibromo-, acetate	292	C8H6Br2O2	036914-79-1	38
5	1-(2-Bromo-2-chloroethenyl)-4-ch...	250	C8H5BrCl2	1000305-36-0	27





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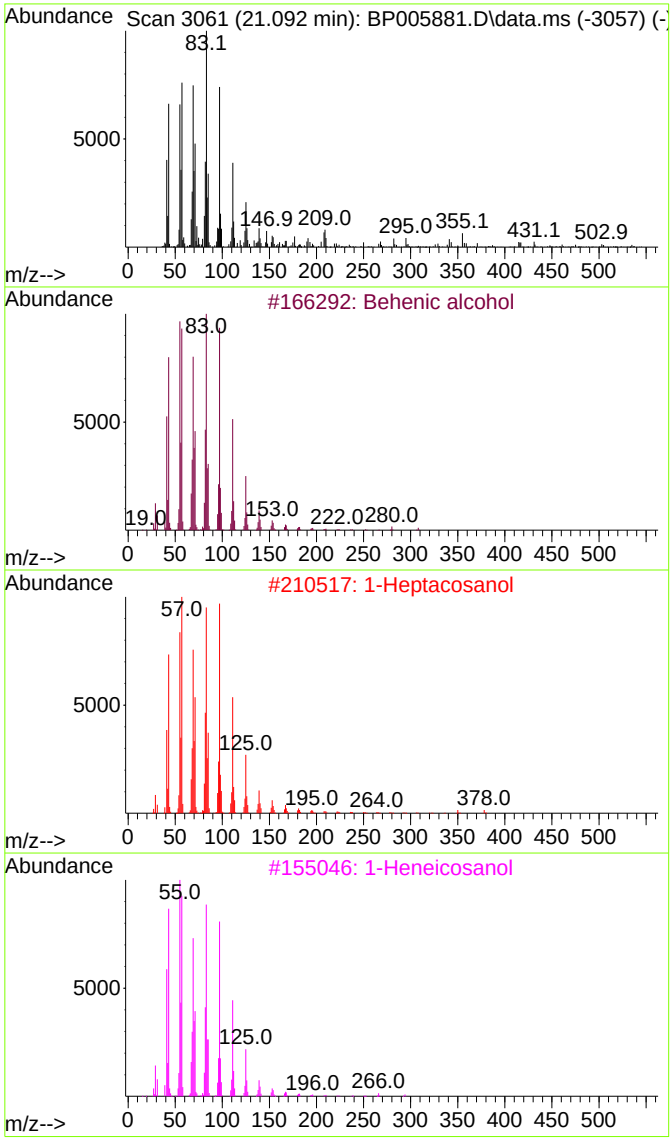
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

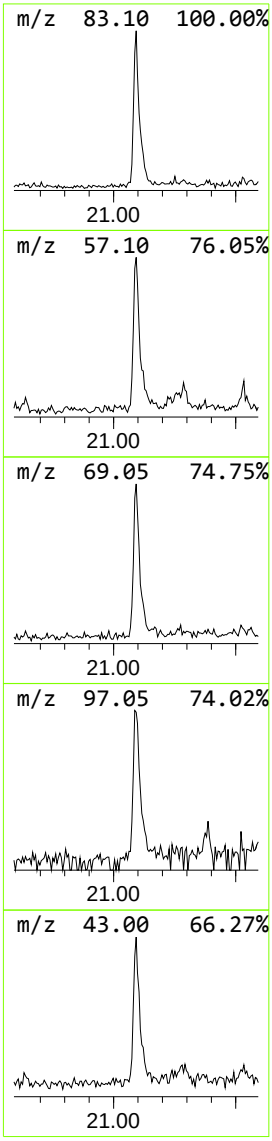
****

Peak Number 8 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.18 ng	115290	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heptacosanol	396	C27H56O	002004-39-9	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Cyclopentadecane	210	C15H30	000295-48-7	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005881.D
Acq On : 11 Jun 2021 20:55
Operator : CG/JU
Sample : M2625-20
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(214-218)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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
3-Penten-2-one,...	4.440	2.0	ng	37722	1	7.946	368758	20.0
2-Pentanone, 4-...	5.046	2.4	ng	44492	1	7.946	368758	20.0
Benzen-d5-amine	7.246	6.1	ng	113126	1	7.946	368758	20.0
2-Cyclohexen-1-...	8.605	7.4	ng	136697	1	7.946	368758	20.0
Ethanol, 2-(2-b...	10.546	3.2	ng	75387	2	10.752	468306	20.0
Cyclohexasiloxa...	12.028	2.9	ng	67342	2	10.752	468306	20.0
Phenol, 2,4-dib...	13.040	2.0	ng	60564	3	14.569	604965	20.0
Behenic alcohol	21.092	2.2	ng	115290	5	21.386	1057720	20.0