LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003598.D
Acq On : 09 Oct 2020 17:47
Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11995

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-BP091520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003598.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.617	289	294	304	rBV	25512	40631	1.55%	0.312%
2	5.099	370	376	401	rBV	552312	954563	36.39%	7.337%
3	6.693	637	647	670	rBV	514327	975855	37.20%	7.501%
4	7.475	774	780	796	rBV	159674	266308	10.15%	2.047%
5	8.628	970	976	1004	rBV	371704	695725	26.52%	5.348%
6	10.252	1245	1252	1264	rBV	196510	347497	13.25%	2.671%
7	12.557	1639	1644	1648	rBV5	32252	53211	2.03%	0.409%
8	12.751	1669	1677	1687	rBV	1175345	1811137	69.04%	13.921%
9	12.910	1700	1704	1709	rBV	60580	85915	3.28%	0.660%
10	13.051	1725	1728	1736	rVB4	26700	49313	1.88%	0.379%
11	13.399	1784	1787	1793	rVB6	55357	88320	3.37%	0.679%
12	13.463	1794	1798	1802	rBV2	41579	65034	2.48%	0.500%
13	13.557	1809	1814	1818	rBV	138299	201828	7.69%	1.551%
14	13.604	1818	1822	1828	rBV	113376	156753	5.98%	1.205%
15	13.875	1864	1868	1873	rBV3	93434	170269	6.49%	1.309%
16	13.969	1880	1884	1888	rVB	210581	285154	10.87%	2.192%
17	14.040	1893	1896	1901	rBV3	53922	90420	3.45%	0.695%
18	14.104	1903	1907	1909	rBV	123429	178818	6.82%	1.374%
19	14.140	1909	1913	1924	rVB	329040	540222	20.59%	4.152%
20	14.234	1925	1929	1933	rBV2	99542	168147	6.41%	1.292%
21	14.804	2023	2026	2030	rVB2	132047	163520	6.23%	1.257%
22	14.934	2044	2048	2054	rBV	347464	492068	18.76%	3.782%
23	15.645	2165	2169	2175	rBV	843473	1290247	49.19%	9.917%
24	19.492	2819	2823	2833	rVB	2124948	2623165	100.00%	20.162%
25	21.016	3078	3082	3086	rVB	475996	601033	22.91%	4.620%
26	23.174	3444	3449	3462	rVB	333201	615012	23.45%	4.727%

Sum of corrected areas: 13010165

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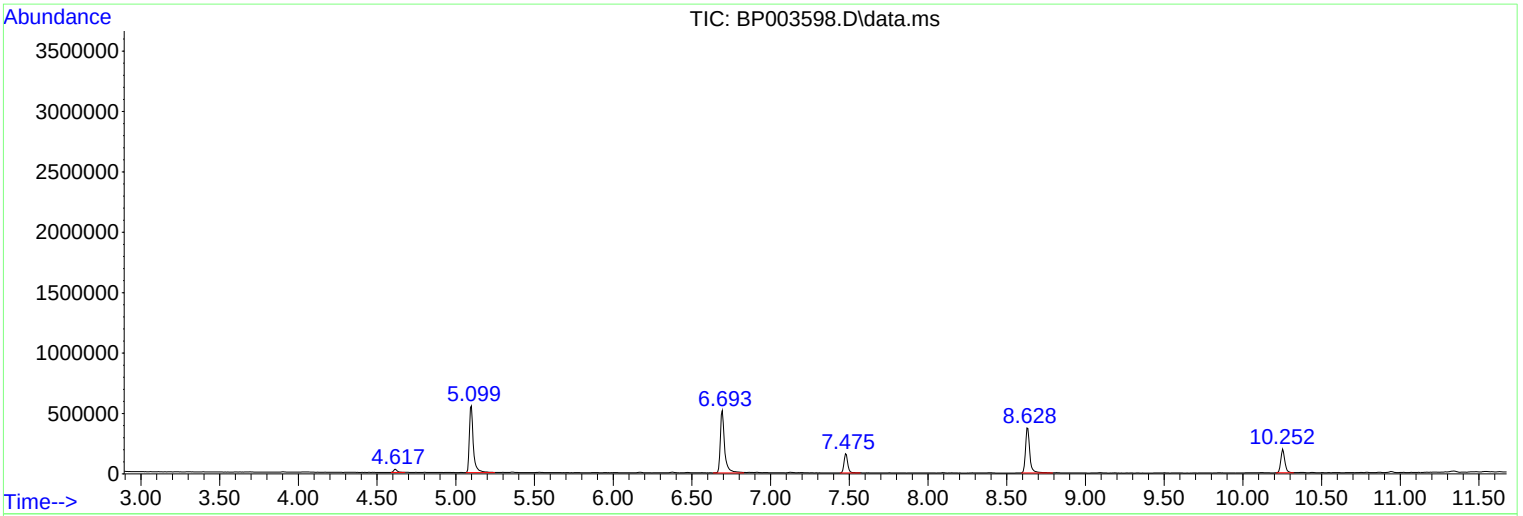
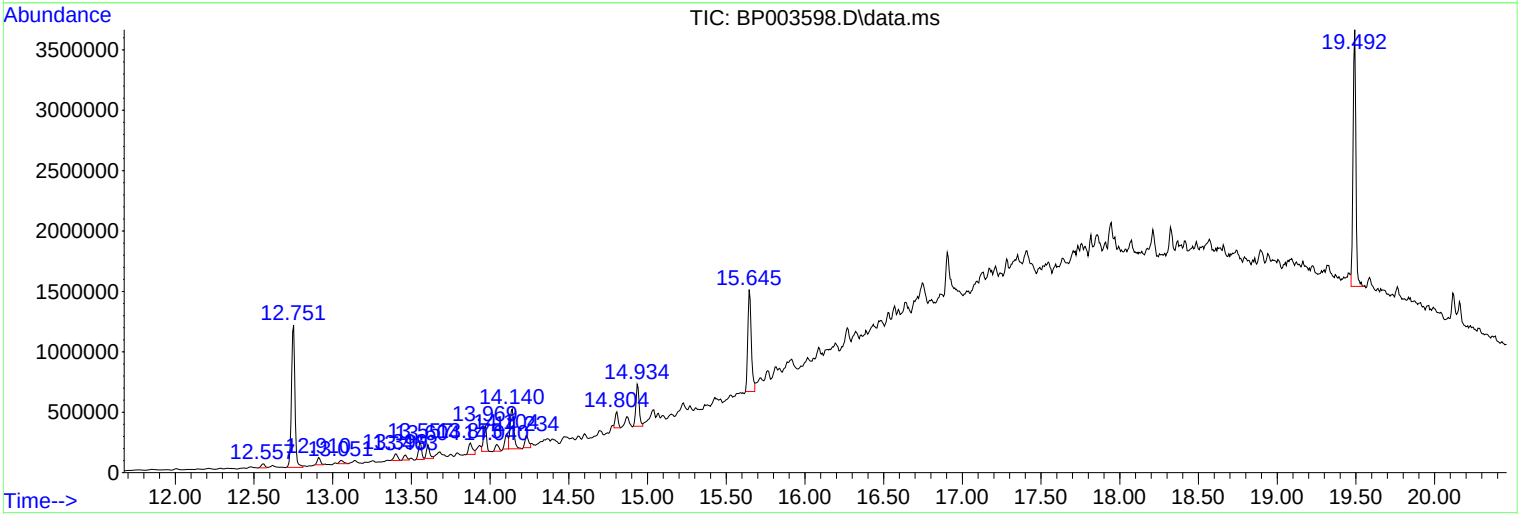
Misc :
ALS Vial : 12 Sample Multiplier: 1

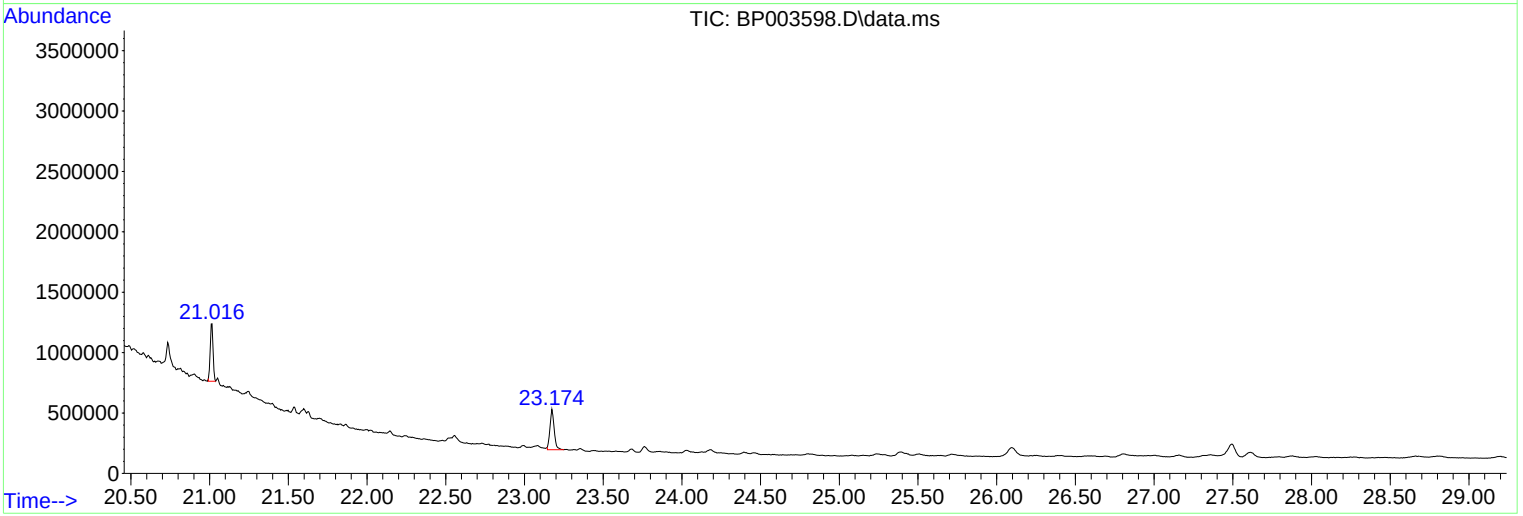
Instrument :
BNA_P
ClientSampleId :
11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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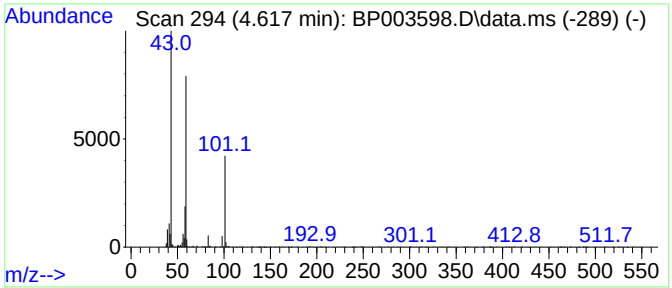
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

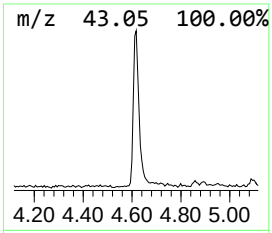
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

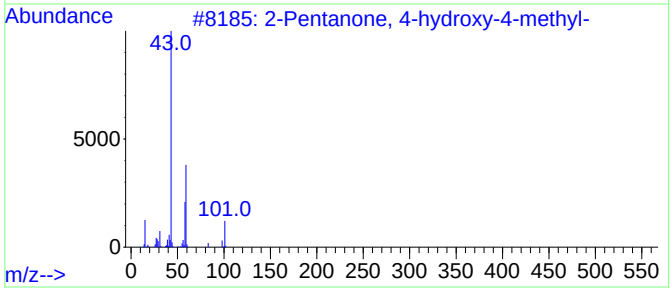
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

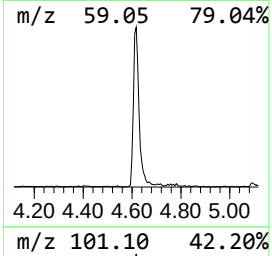
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.617	3.05 ng	40631	1,4-Dichlorobenzene-d4	7.475

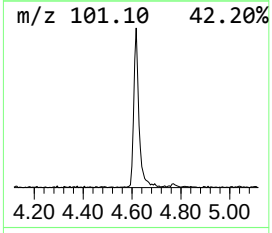
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	45
3	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	25
4	1,2-Butanediol	90	C4H10O2	000584-03-2	25
5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	23

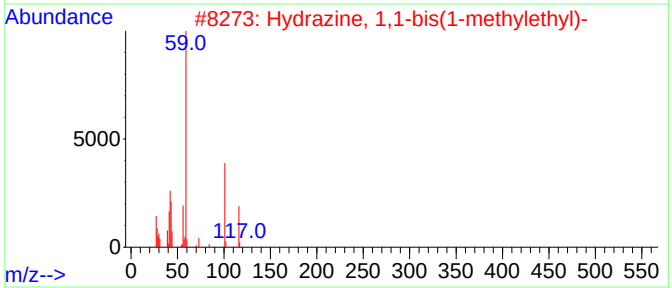


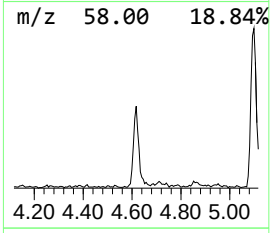


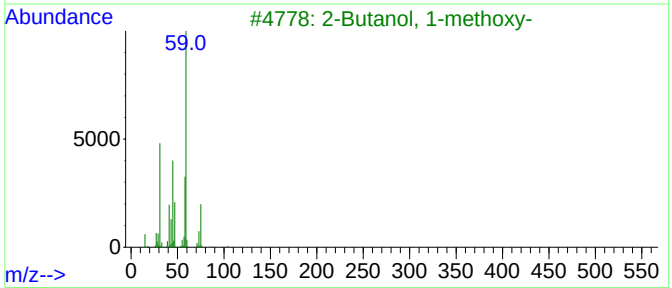


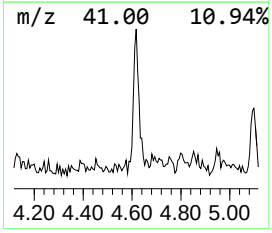












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Data File : BP003598.D
Acq On : 09 Oct 2020 17:47
Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

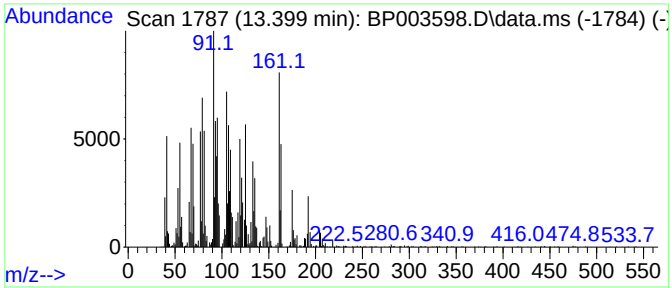
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

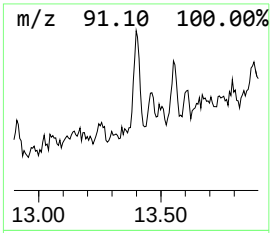
****

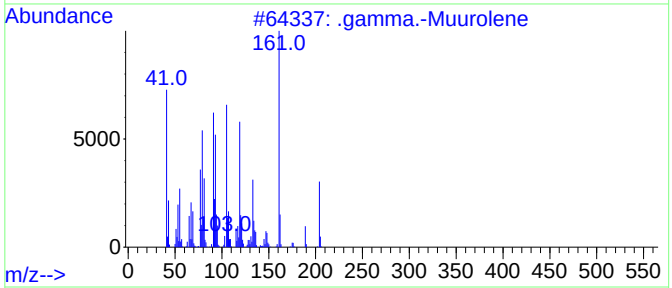
Peak Number 3 .gamma.-Muurolene Concentration Rank 7

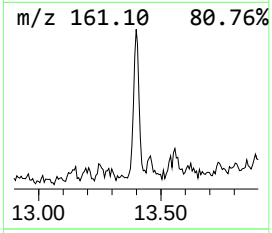
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.399	3.27 ng	88320	Acenaphthene-d10	14.140

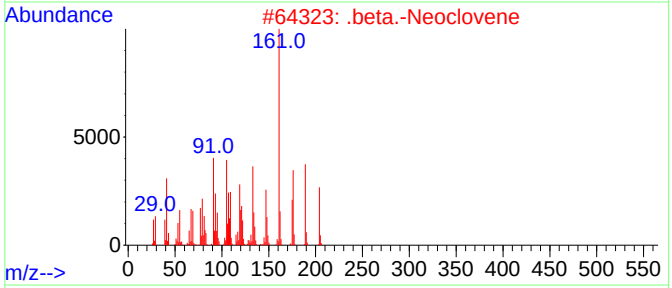
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Muurolene	204	C15H24	030021-74-0	83
2	.beta.-Neoclovene	204	C15H24	056684-96-9	55
3	Longifolene	204	C15H24	000475-20-7	50
4	Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	42
5	Cyclohexene, 6-ethenyl-6-methyl-...	204	C15H24	005951-67-7	38

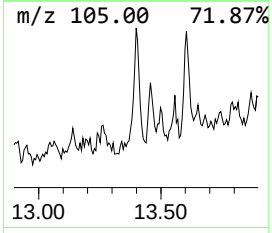


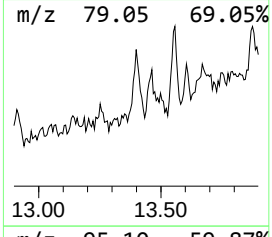


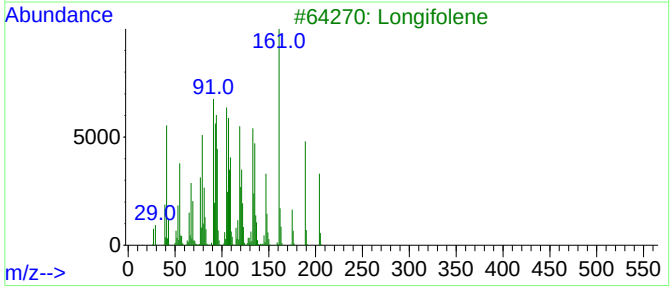


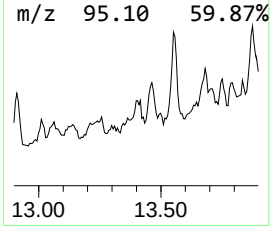












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Data File : BP003598.D
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Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

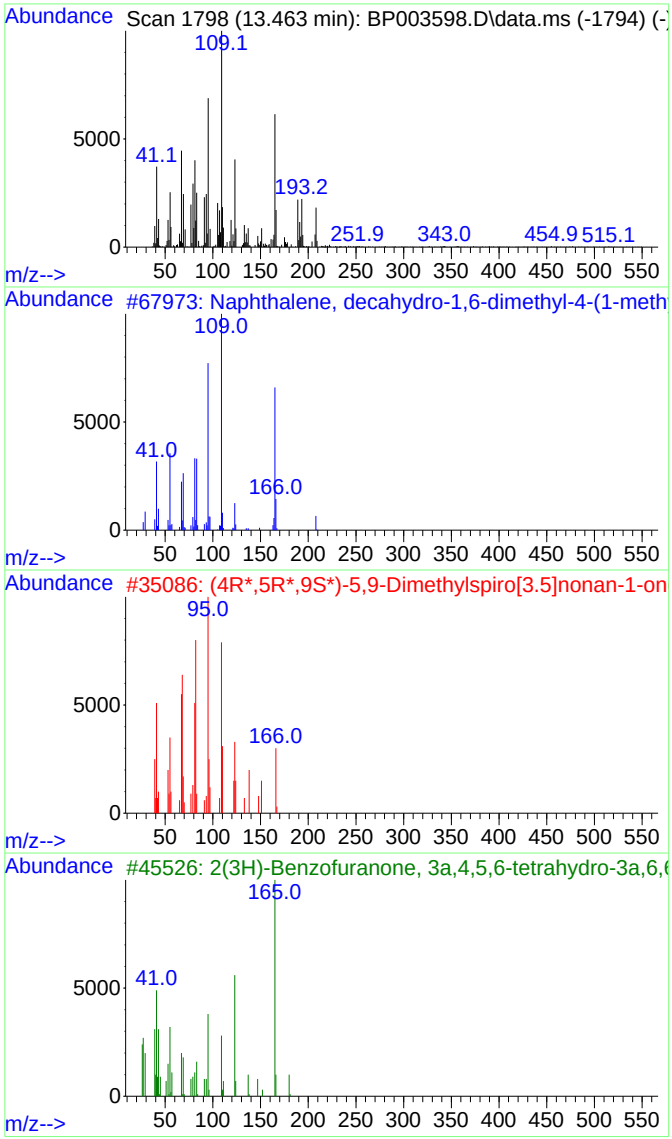
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

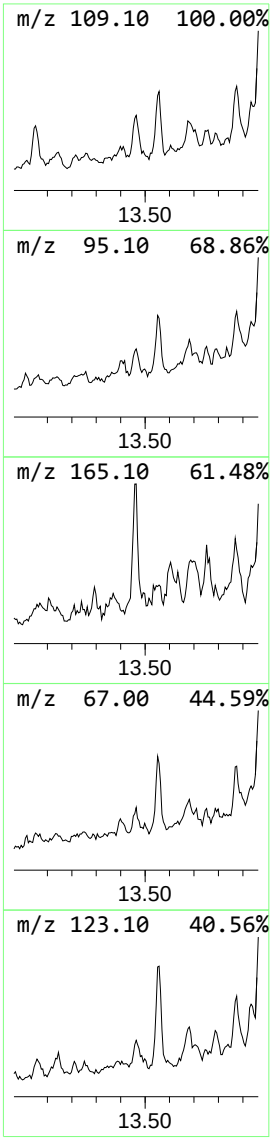
****

Peak Number 4 unknown13.46 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	2.41 ng	65034	Acenaphthene-d10	14.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	47
2	(4R*,5R*,9S*)-5,9-Dimethylspiro[...	166	C11H18O	063088-19-7	30
3	2(3H)-Benzofuranone, 3a,4,5,6-te...	180	C11H16O2	016778-26-0	27
4	2,5-Furandione, dihydro-3-(2-met...	154	C8H10O3	018908-20-8	27
5	Benzenamine, 4-(hexyloxy)-	193	C12H19NO	039905-57-2	22





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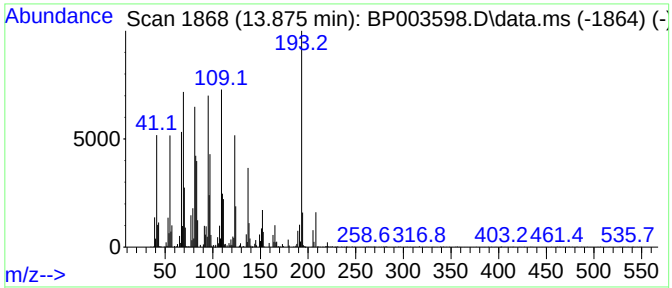
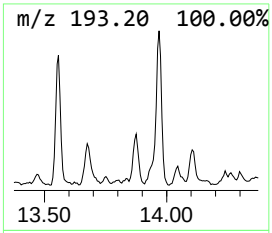
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

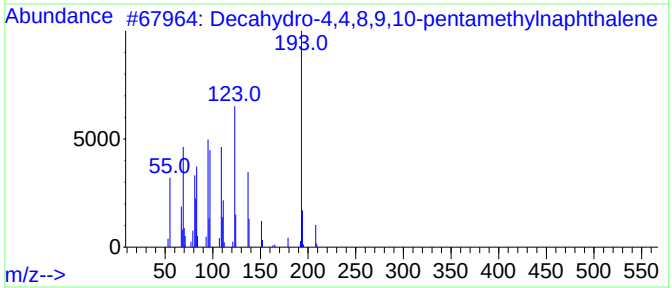
****
Peak Number 5 Decahydro-4,4,8,9,10-pentam... Concentration Rank 3

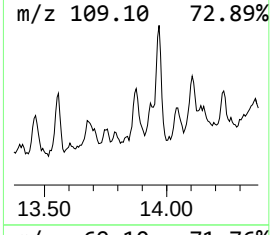
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.875	6.30 ng	170269	Acenaphthene-d10	14.140

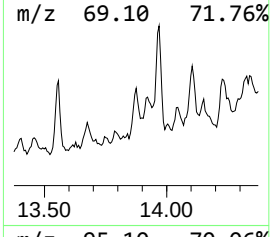
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	97
2	1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	50
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	43
4	2-Phenylindolizine	193	C14H11N	025379-20-8	38
5	1-Anthracenamine	193	C14H11N	000610-49-1	38

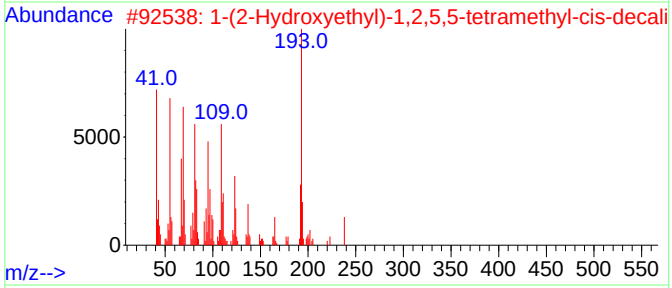


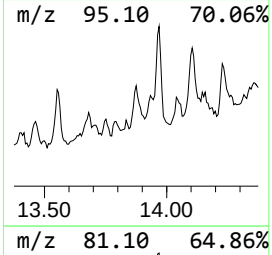


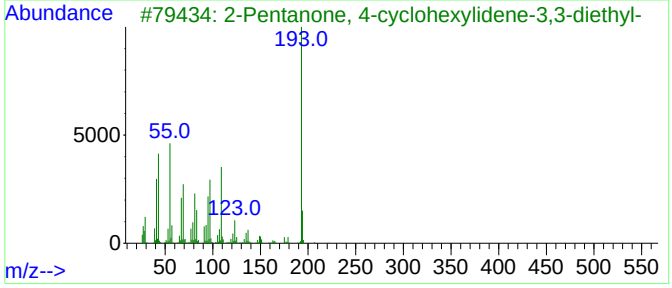


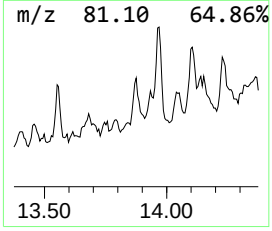












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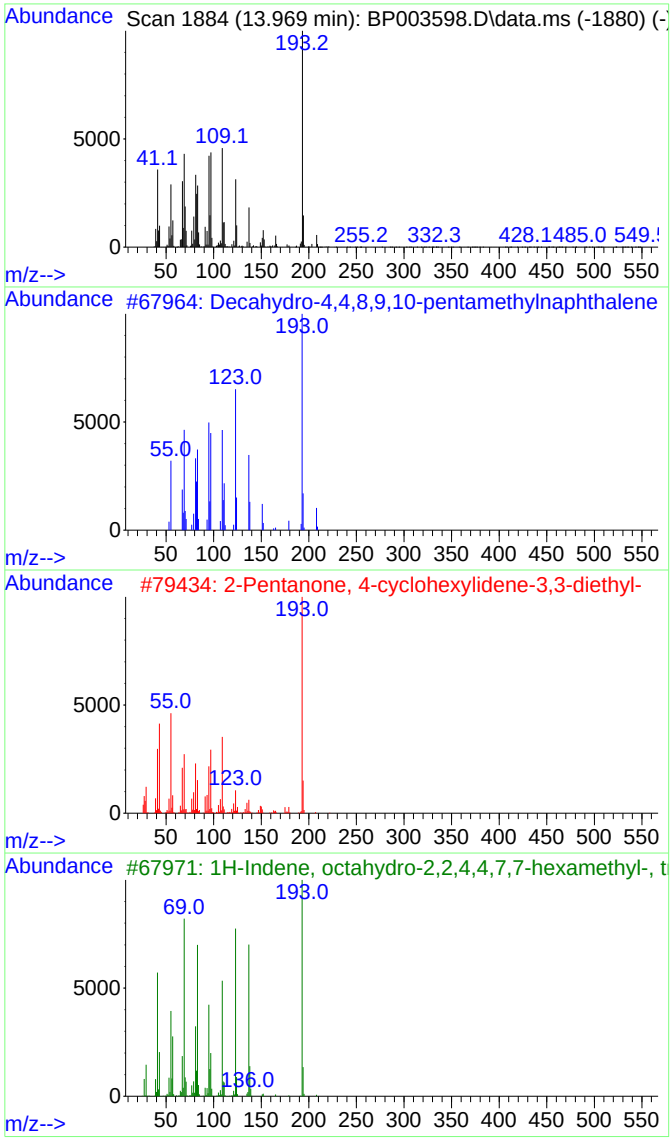
TIC Integration Parameters: LSCINT.P

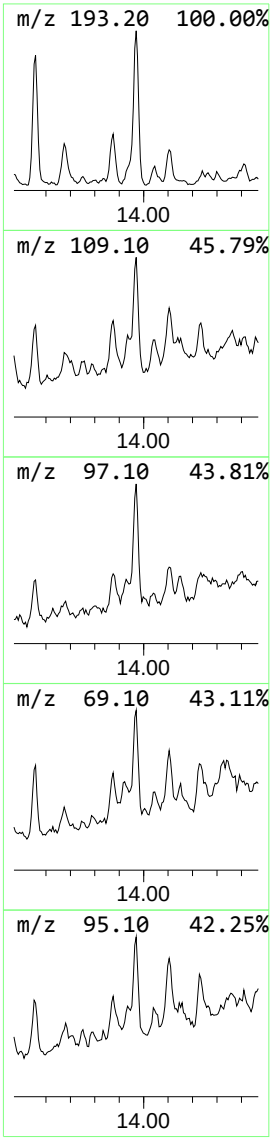
****

Peak Number 6 unknown13.96 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	10.56 ng	285154	Acenaphthene-d10	14.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	64
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	37
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
5	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22





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Data File : BP003598.D
Acq On : 09 Oct 2020 17:47
Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

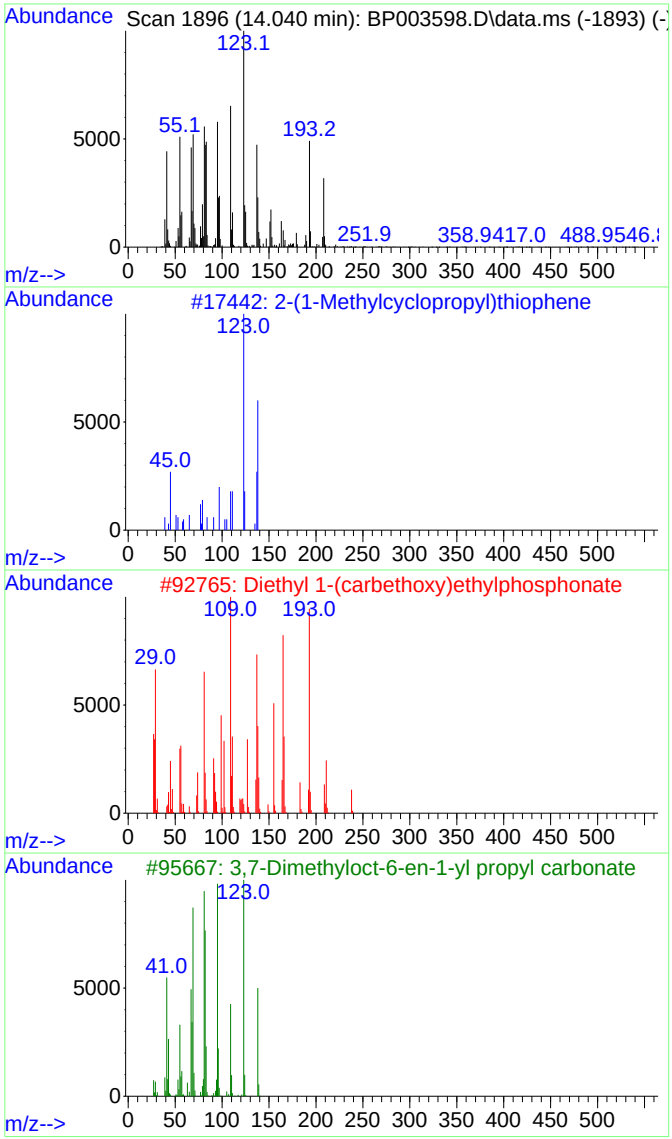
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

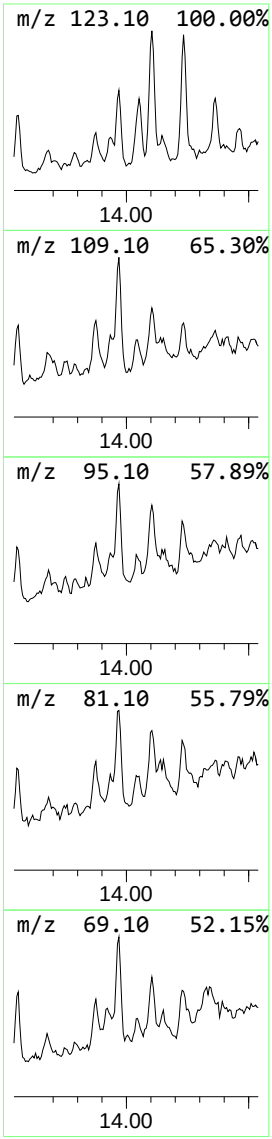
****

Peak Number 7 unknown14.04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.040	3.35 ng	90420	Acenaphthene-d10	14.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Methylcyclopropyl)thiophene	138	C8H10S	1000100-02-7	35
2	Diethyl 1-(carbethoxy)ethylphosp...	238	C9H19O5P	1000306-25-7	30
3	3,7-Dimethyloct-6-en-1-yl propyl...	242	C14H26O3	1000372-83-5	27
4	Naphthalene, decahydro-1,8a-dime...	208	C15H28	015404-63-4	25
5	10.alpha.-Eremophilane	208	C15H28	003242-05-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003598.D
Acq On : 09 Oct 2020 17:47
Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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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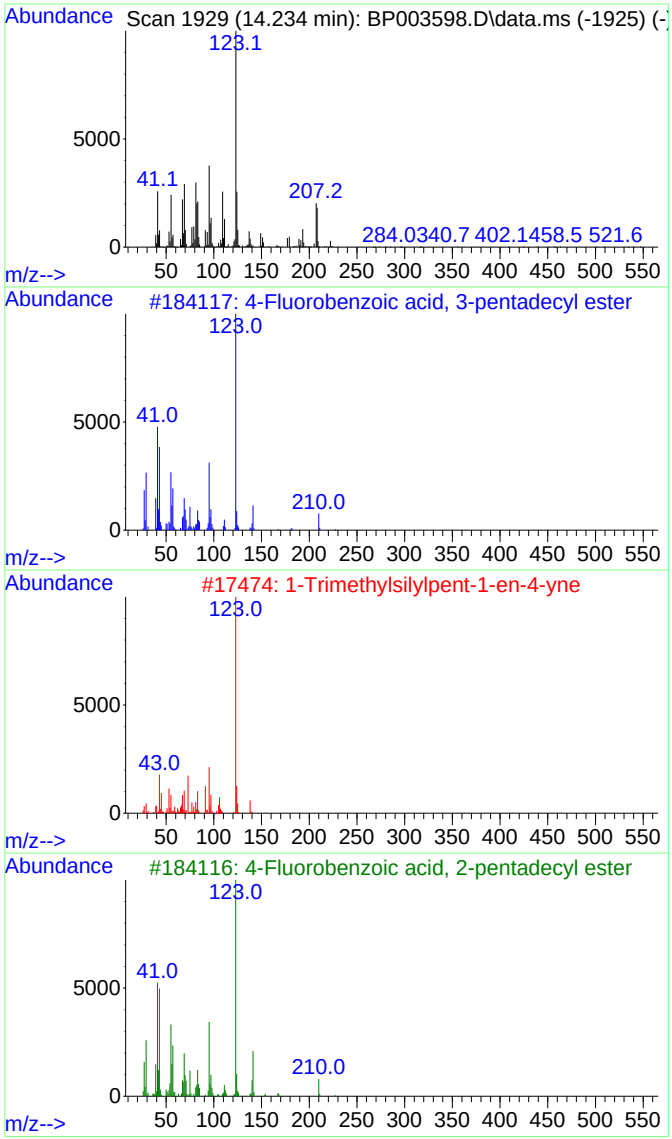
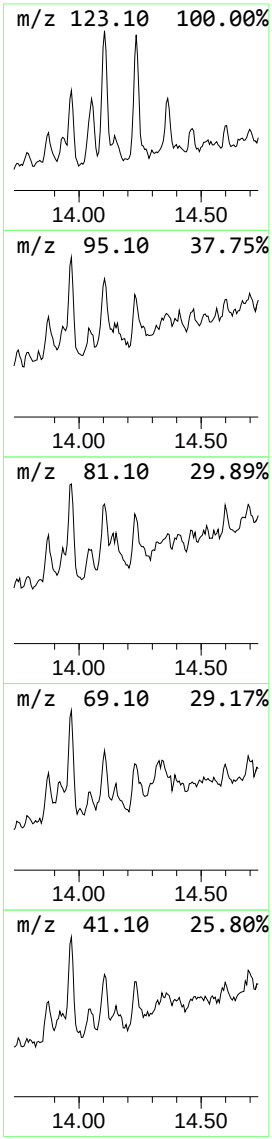
Peak Number 8 unknown14.23 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.234	6.23 ng	168147	Acenaphthene-d10	14.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	47
2	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	47
3	4-Fluorobenzoic acid, 2-pentadec...	350	C22H35FO2	1000280-68-3	38
4	Pyridine, 1,2,3,6-tetrahydro-1-(...	153	C9H15NO	057150-46-6	38
5	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1000215-77-9	38





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Data File : BP003598.D
Acq On : 09 Oct 2020 17:47
Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11995

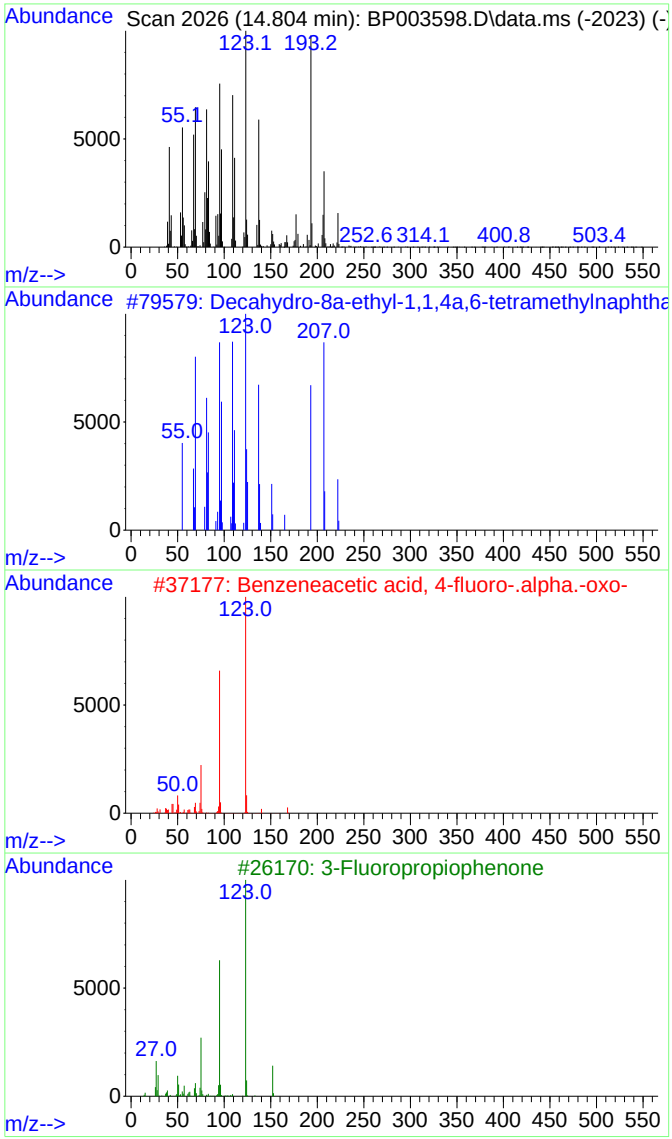
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

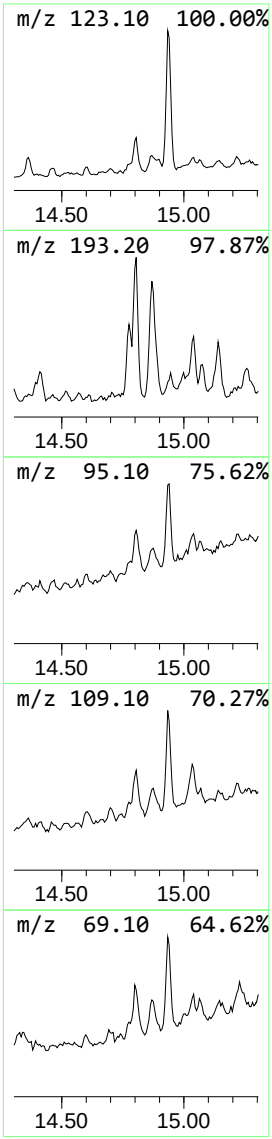
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	6.05 ng	163520	Acenaphthene-d10	14.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	70
2	Benzeneacetic acid, 4-fluoro-.al...	168	C8H5FO3	002251-76-5	22
3	3-Fluoropropiophenone	152	C9H9FO	000455-67-4	22
4	Pyrazolo[5,1-c]-as-triazine-3-ca...	193	C6H7N7O	016111-78-7	22
5	2-Fluorobenzoic acid, 3,5-dimeth...	250	C15H19FO2	1000278-96-6	22





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Data File : BP003598.D
Acq On : 09 Oct 2020 17:47
Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
11995

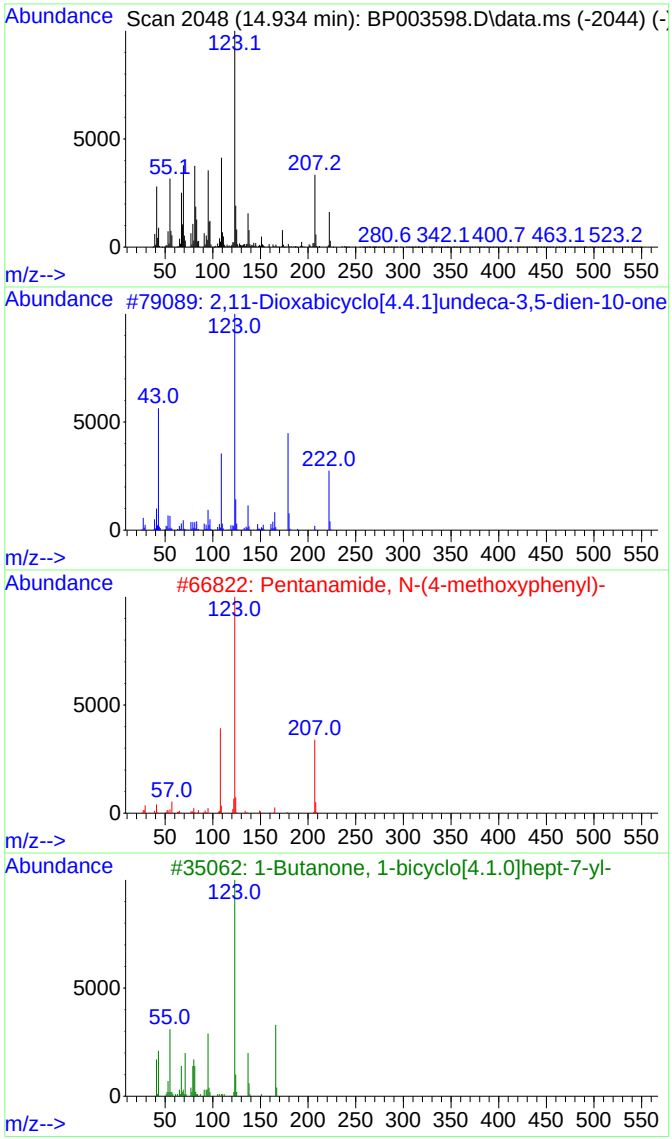
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

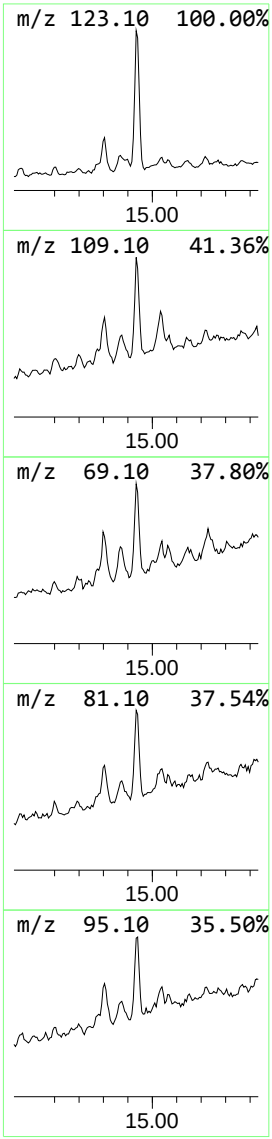
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.934	18.22 ng	492068	Acenaphthene-d10	14.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	53
2	Pentanamide, N-(4-methoxyphenyl)-	207	C12H17NO2	1000306-89-3	43
3	1-Butanone, 1-bicyclo[4.1.0]hept...	166	C11H18O	054764-62-4	43
4	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	43
5	1-(1-Ethyl-2,3-dimethyl-cyclopen...	166	C11H18O	1000185-18-6	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003598.D
Acq On : 09 Oct 2020 17:47
Operator : CG/JU
Sample : L4319-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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
2-Pentanone, 4-...	4.617	3.0	ng	40631	1	7.475	266308	20.0
.gamma.-Muurolene	13.399	3.3	ng	88320	3	14.140	540222	20.0
unknown13.46	13.463	2.4	ng	65034	3	14.140	540222	20.0
Decahydro-4,4,8...	13.875	6.3	ng	170269	3	14.140	540222	20.0
unknown13.96	13.969	10.6	ng	285154	3	14.140	540222	20.0
unknown14.04	14.040	3.4	ng	90420	3	14.140	540222	20.0
unknown14.23	14.234	6.2	ng	168147	3	14.140	540222	20.0
Decahydro-8a-et...	14.804	6.0	ng	163520	3	14.140	540222	20.0
2,11-Dioxabicyc...	14.934	18.2	ng	492068	3	14.140	540222	20.0