LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028469.D
Acq On : 20 Jan 2021 15:53
Operator : CG/JU
Sample : M1124-01
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument : BNA_M
ClientSampleId : VNJ-231

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_M\Methods\8270-BM012021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028469.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.551	396	402	414	rBV	385653	590675	47.16%	5.933%
2	7.187	673	680	690	rVB	394507	636922	50.85%	6.398%
3	8.034	817	824	832	rBV	228651	362742	28.96%	3.644%
4	9.204	1017	1023	1030	rVB	256015	418246	33.39%	4.201%
5	10.851	1296	1303	1309	rVB	292789	494422	39.48%	4.967%
6	13.298	1713	1719	1725	rVB	607584	879272	70.20%	8.833%
7	13.457	1742	1746	1748	rBV2	47920	70806	5.65%	0.711%
8	14.092	1850	1854	1858	rBV2	222017	335230	26.77%	3.367%
9	14.198	1868	1872	1882	rBV4	176392	325070	25.95%	3.265%
10	14.316	1889	1892	1896	rBV4	115065	148549	11.86%	1.492%
11	14.410	1903	1908	1913	rBV6	181593	404217	32.27%	4.060%
12	14.498	1919	1923	1929	rVB	427443	663455	52.97%	6.665%
13	14.633	1942	1946	1949	rBV3	219750	397558	31.74%	3.994%
14	14.674	1949	1953	1959	rVB3	528678	878027	70.10%	8.820%
15	15.186	2036	2040	2044	rBV3	311932	502938	40.16%	5.052%
16	15.457	2081	2086	2090	rBV3	796593	1252446	100.00%	12.581%
17	21.539	3116	3120	3124	rVB	640954	777242	62.06%	7.808%
18	23.815	3502	3507	3520	rVB2	408730	817103	65.24%	8.208%

Sum of corrected areas: 9954920

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
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Operator : CG/JU
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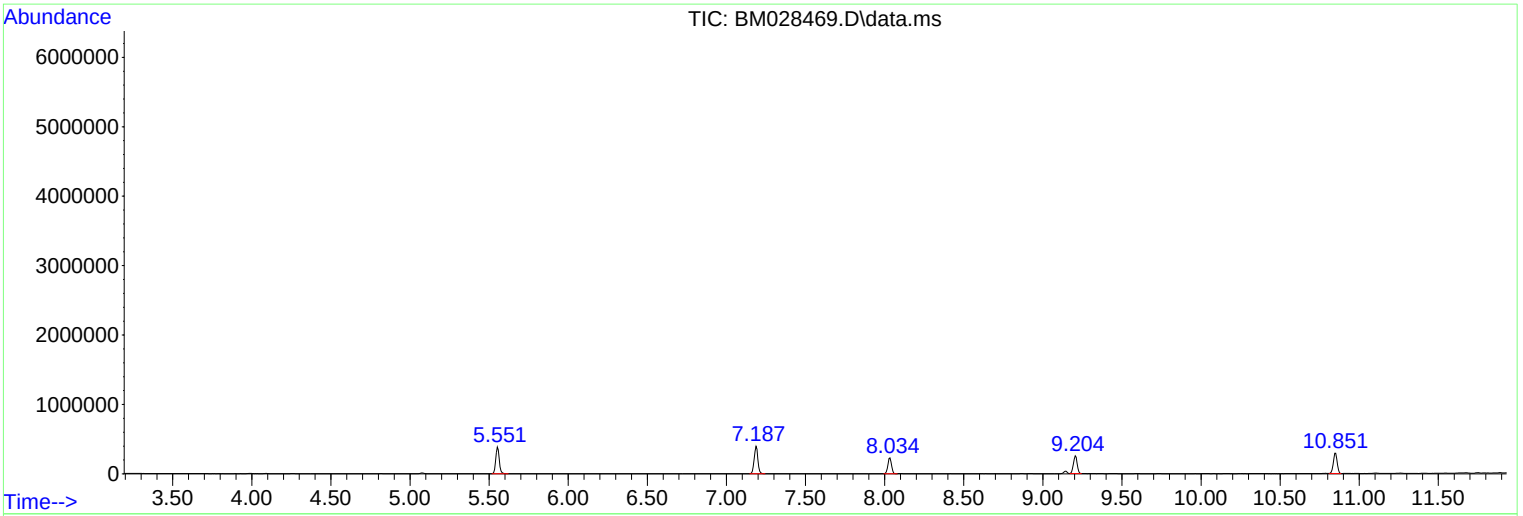
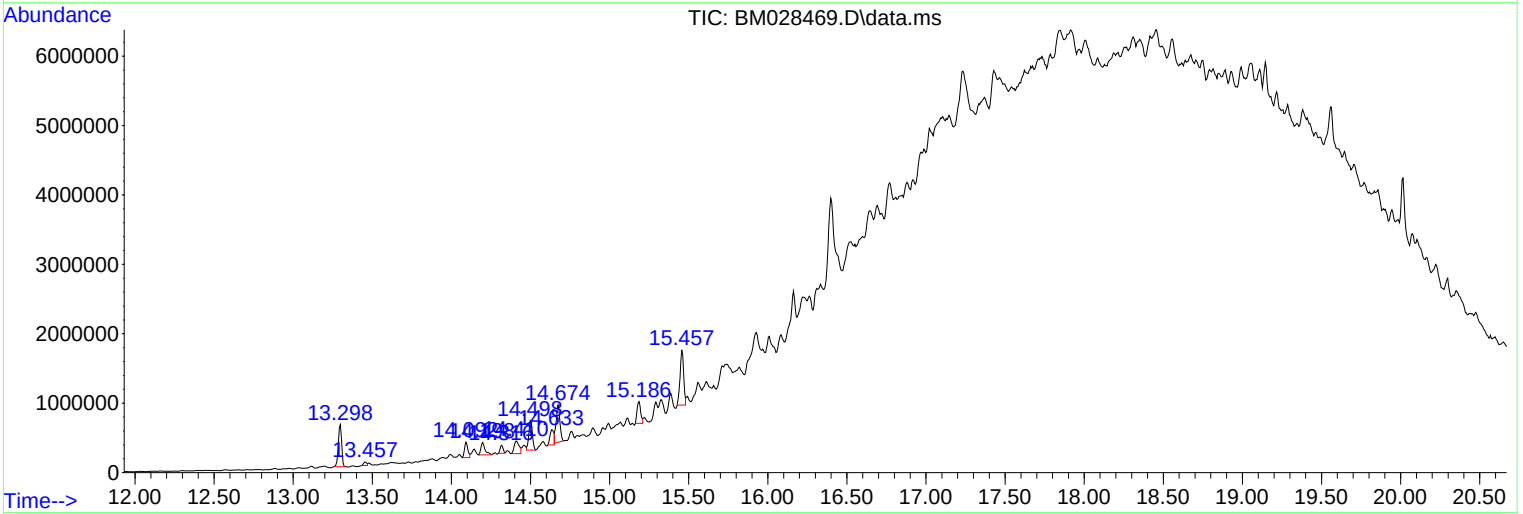
Misc :
ALS Vial : 11 Sample Multiplier: 2

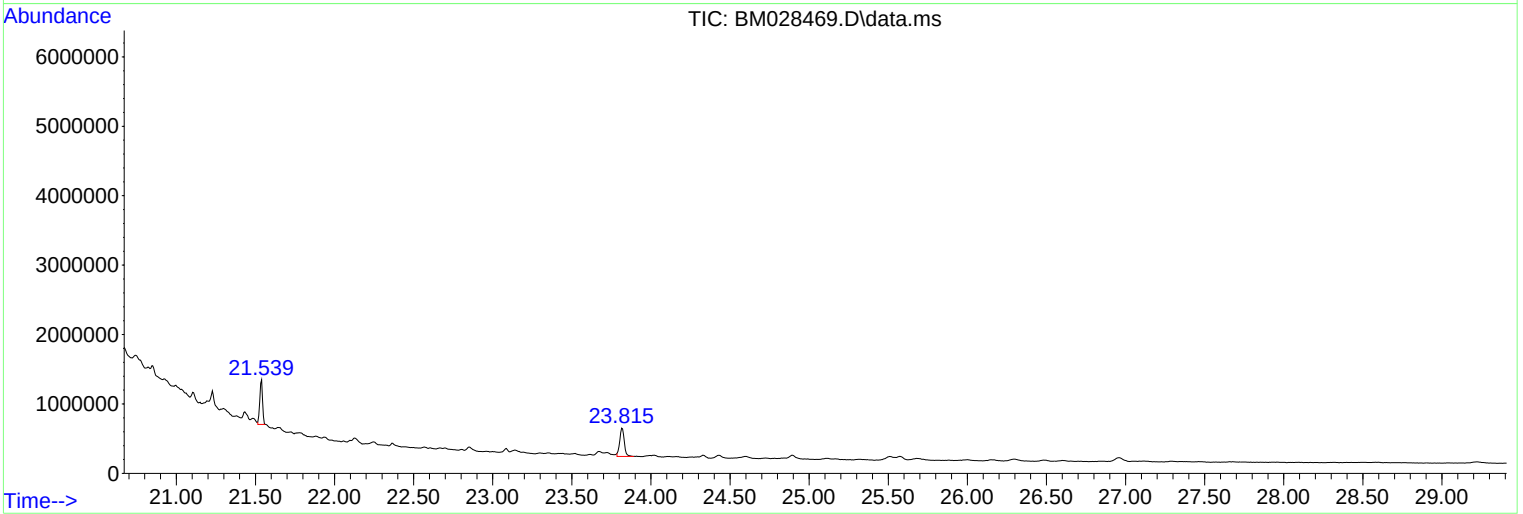
Instrument :
BNA_M
ClientSampleId :
VNJ-231

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028469.D
Acq On : 20 Jan 2021 15:53
Operator : CG/JU
Sample : M1124-01
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument :
BNA_M
ClientSampleId :
VNJ-231

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

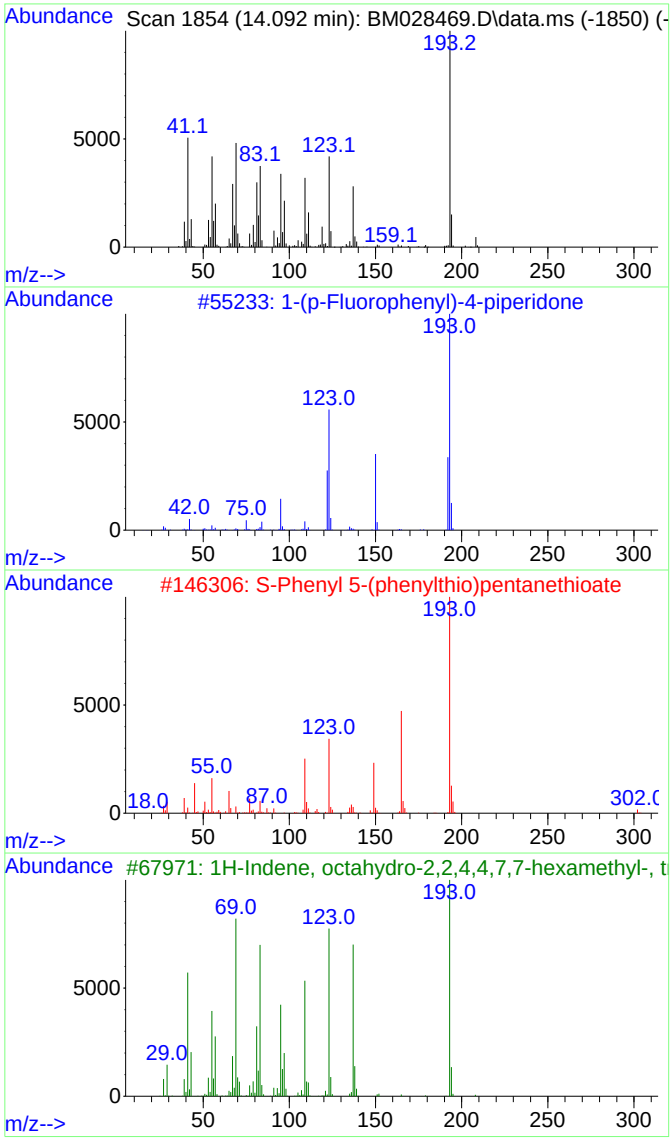
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

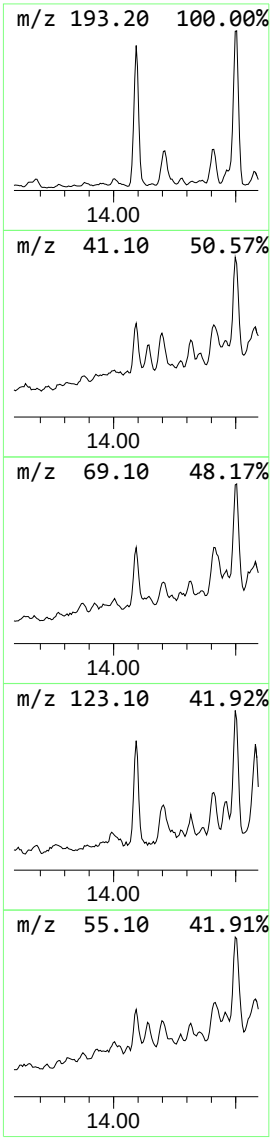
****

Peak Number 1 unknown14.092 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.092	7.64 ng	335230	Acenaphthene-d10	14.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	47
2	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	40
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
4	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
5	Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028469.D
Acq On : 20 Jan 2021 15:53
Operator : CG/JU
Sample : M1124-01
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument : BNA_M
ClientSampleId : VNJ-231

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

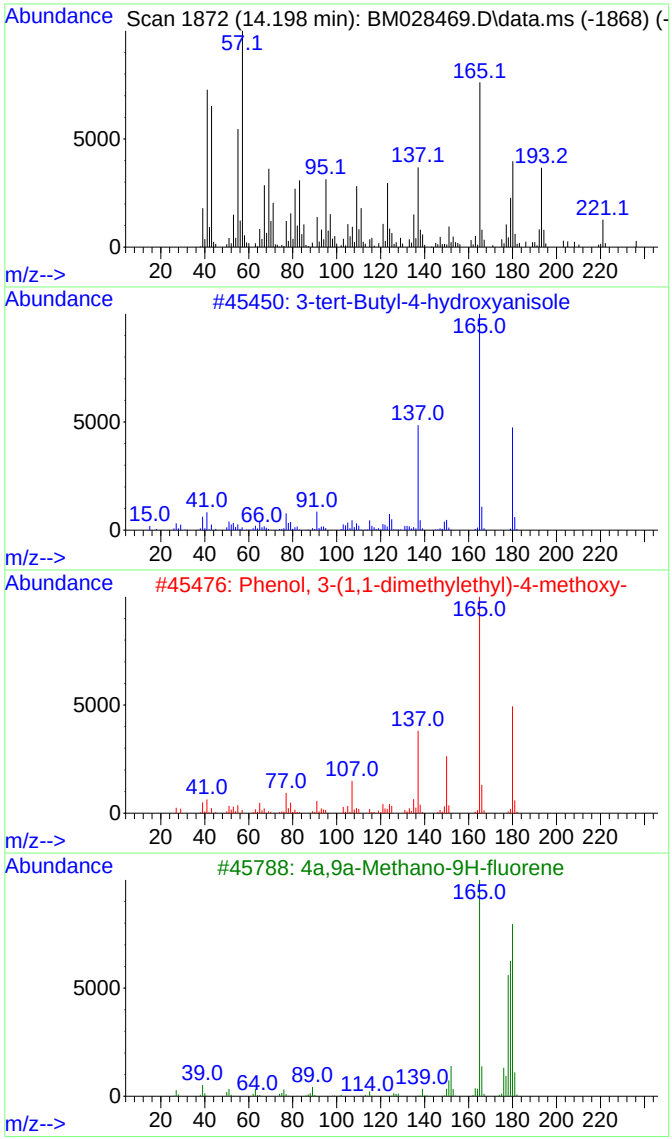
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

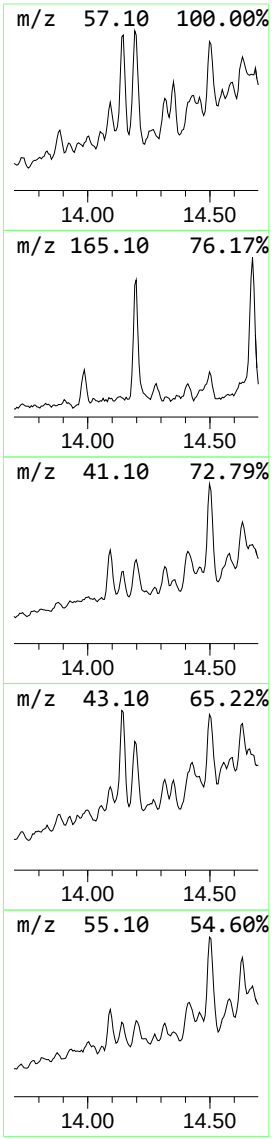
****

Peak Number 2 unknown14.198 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	7.40 ng	325070	Acenaphthene-d10	14.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	49
2	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	46
3	4a,9a-Methano-9H-fluorene	180	C14H12	019540-84-2	46
4	Pentacyclo[6.4.0.1(1,8).1(2,7)]t...	180	C14H12	086120-84-5	46
5	Ethanone, 1-(2,5-dimethoxyphenyl)-	180	C10H12O3	001201-38-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028469.D
Acq On : 20 Jan 2021 15:53
Operator : CG/JU
Sample : M1124-01
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument : BNA_M
ClientSampleId : VNJ-231

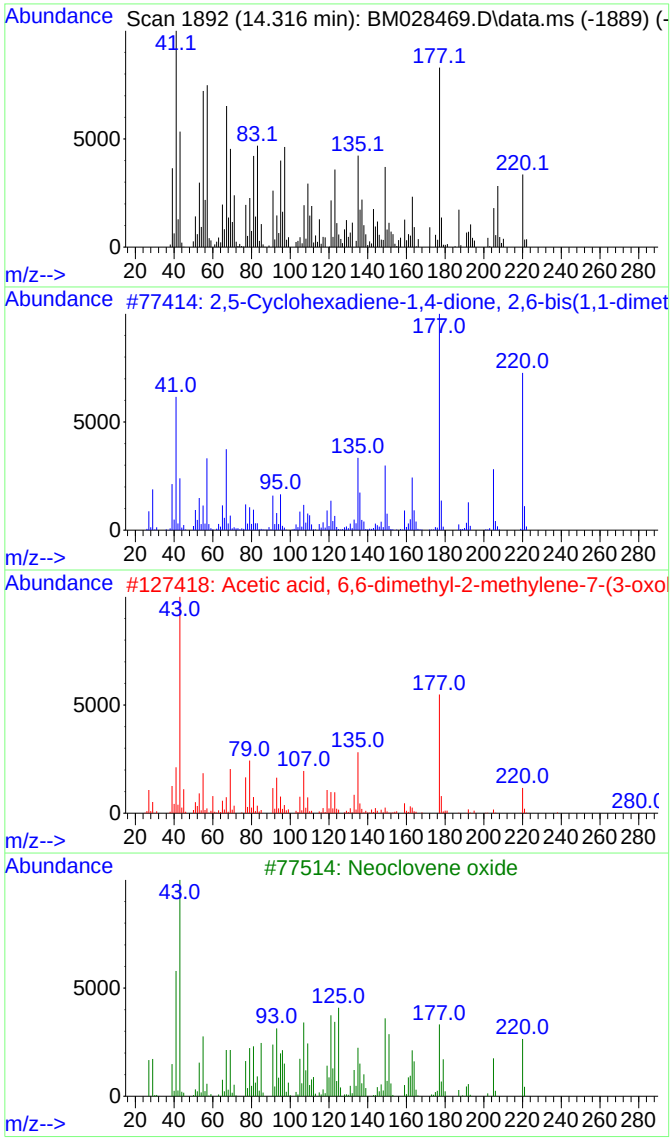
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

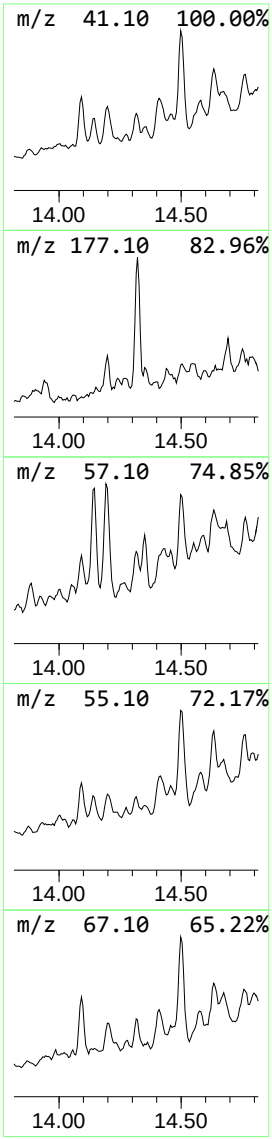
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.316	3.38 ng	148549	Acenaphthene-d10	14.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	Acetic acid, 6,6-dimethyl-2-meth...	280	C16H24O4	1000186-15-5	35
3	Neoclovene oxide	220	C15H24O	1000163-73-4	30
4	Acetic acid, 2,6,6-trimethyl-3-m...	280	C16H24O4	1000185-41-4	27
5	2(1H)-Pyridinone, 1-isopropyl-	137	C8H11NO	022973-00-8	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028469.D
Acq On : 20 Jan 2021 15:53
Operator : CG/JU
Sample : M1124-01
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument : BNA_M
ClientSampleId : VNJ-231

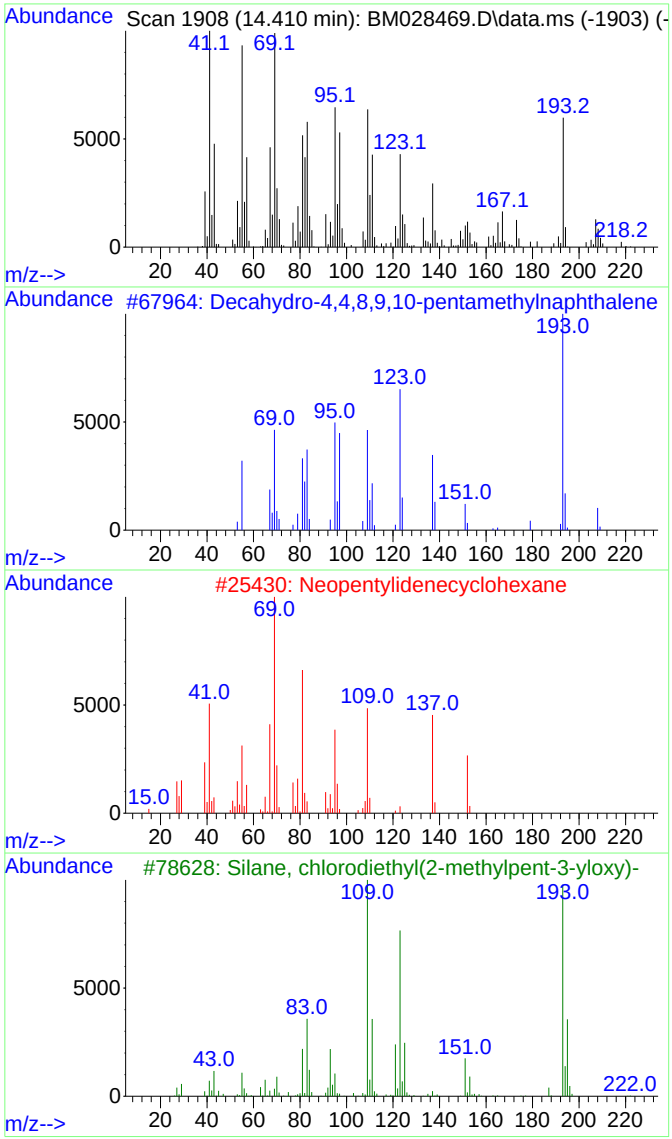
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

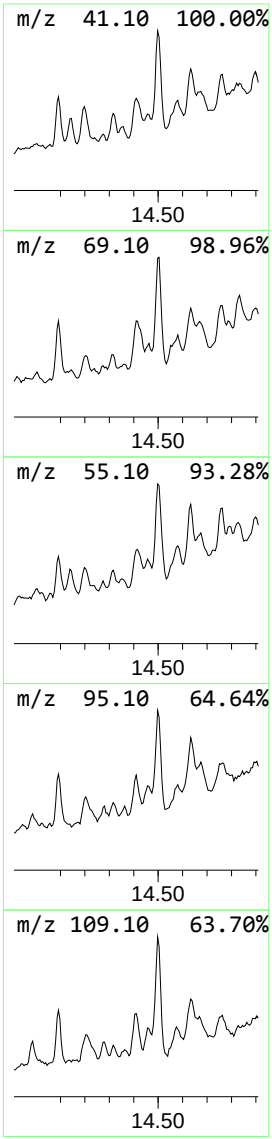
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.410	9.21 ng	404217	Acenaphthene-d10	14.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	93
2	Neopentylidenecyclohexane	152	C11H20	039546-80-0	46
3	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	38
4	1,1'-Bicyclohexyl, 2-ethyl-, cis-	194	C14H26	050991-12-3	35
5	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
Data File : BM028469.D
Acq On : 20 Jan 2021 15:53
Operator : CG/JU
Sample : M1124-01
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument : BNA_M
ClientSampleId : VNJ-231

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

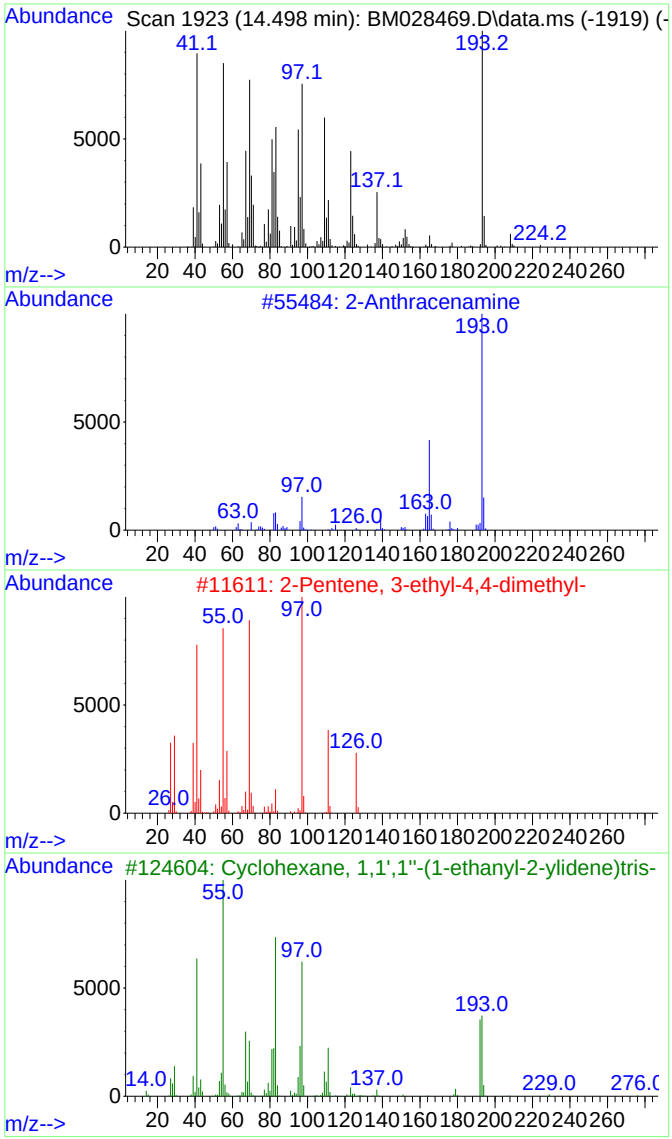
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

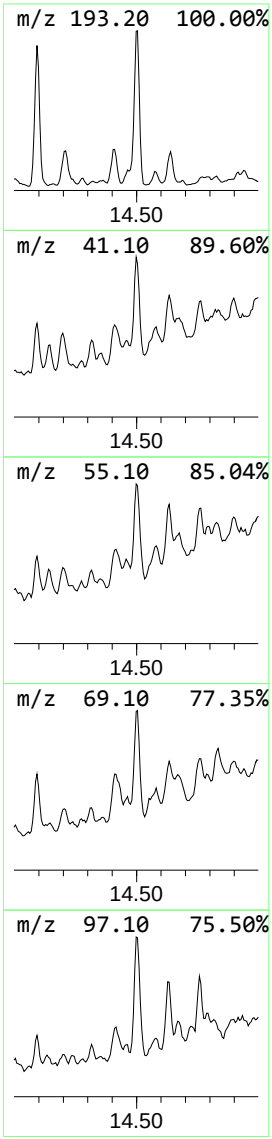
****

Peak Number 5 unknown14.498 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	15.11 ng	663455	Acenaphthene-d10	14.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Anthracenamine	193	C14H11N	000613-13-8	41
2	2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	30
3	Cyclohexane, 1,1',1''-(1-ethanyl...	276	C20H36	055682-86-5	27
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	25
5	Cyclopentanecarboxylic acid, 3-t...	310	C20H38O2	1000280-58-8	22





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Data File : BM028469.D
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Operator : CG/JU
Sample : M1124-01
Misc :
ALS Vial : 11 Sample Multiplier: 2

Instrument : BNA_M
ClientSampleId : VNJ-231

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

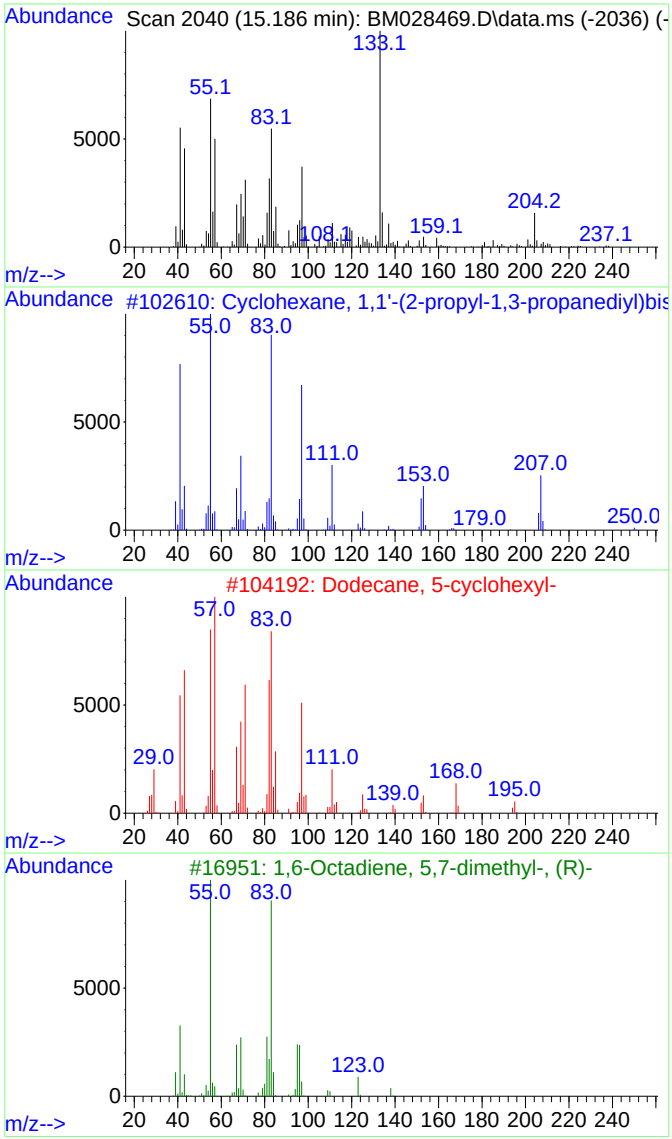
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

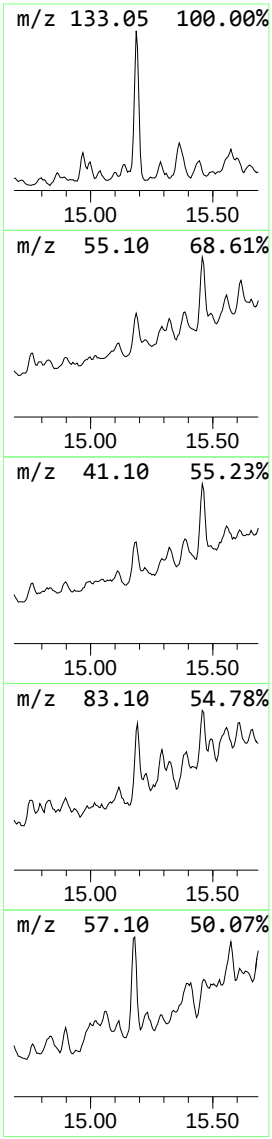
****

Peak Number 6 unknown15.186 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	11.46 ng	502938	Acenaphthene-d10	14.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	27
2	Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	25
3	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	14
4	Cyclododecanol, 1-ethenyl-	210	C14H26O	006244-49-1	11
5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	11





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Sample : M1124-01
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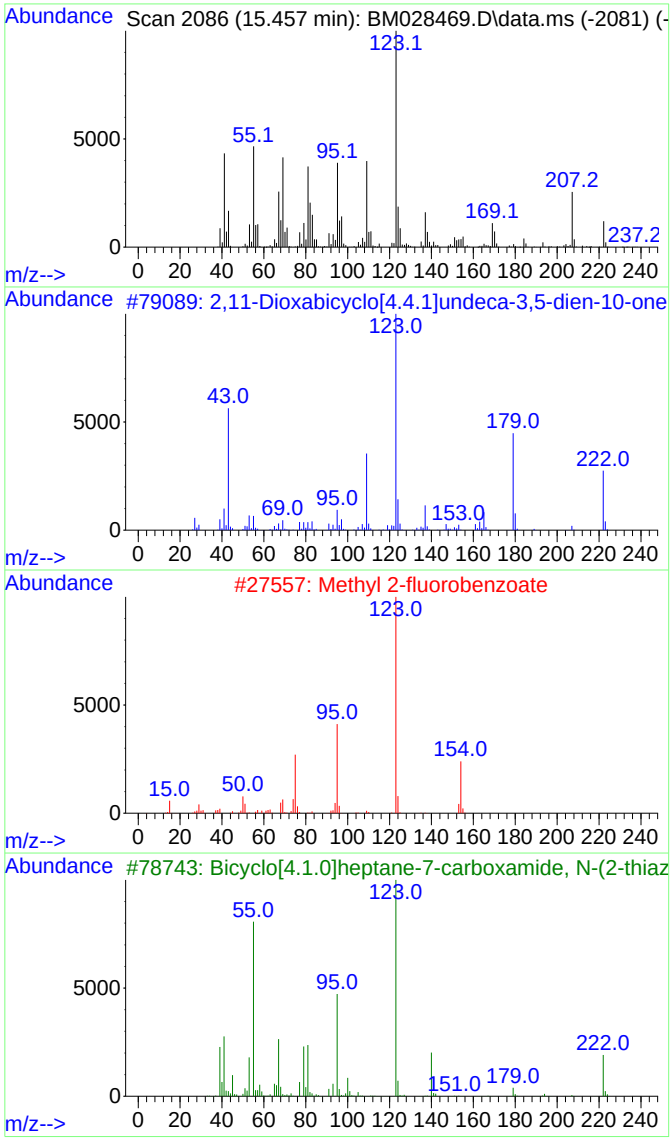
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

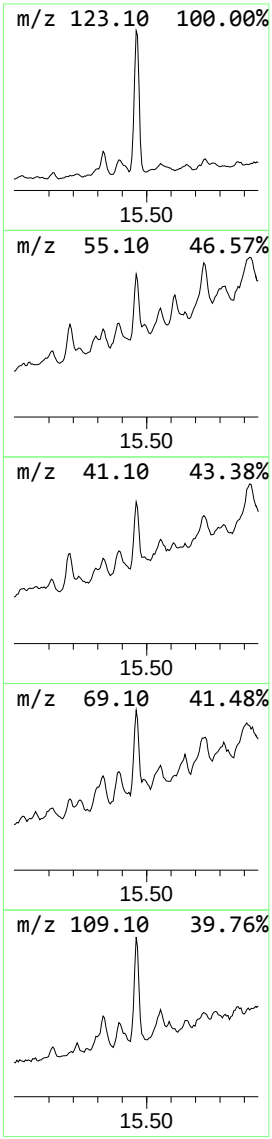
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.457	28.53 ng	1252450	Acenaphthene-d10	14.674

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	50
2	Methyl 2-fluorobenzoate	154	C8H7FO2	000394-35-4	43
3	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	43
4	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	43
5	4-Fluorobenzoic acid, pentafluor...	306	C13H4F6O2	1000355-67-4	43





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown14.092	14.092	7.6	ng	335230	3	14.674	878027	20.0
unknown14.198	14.198	7.4	ng	325070	3	14.674	878027	20.0
2,5-Cyclohexadi...	14.316	3.4	ng	148549	3	14.674	878027	20.0
Decahydro-4,4,8...	14.410	9.2	ng	404217	3	14.674	878027	20.0
unknown14.498	14.498	15.1	ng	663455	3	14.674	878027	20.0
unknown15.186	15.186	11.5	ng	502938	3	14.674	878027	20.0
2,11-Dioxabicyc...	15.457	28.5	ng	1252450	3	14.674	878027	20.0