LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
Data File : BM047438.D
Acq On : 04 Sep 2024 14:44
Operator : RC/JU
Sample : P3820-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
STONE-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_M\Methods\8270-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047438.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	350	360	371	rBV	1526483	2565900	46.12%	8.345%
2	6.569	620	626	641	rVB	1327049	2416459	43.44%	7.859%
3	7.340	746	757	765	rBV	882244	1472742	26.47%	4.790%
4	8.492	947	953	966	rBV	968128	1716120	30.85%	5.581%
5	10.098	1214	1226	1234	rBV	1025079	1790985	32.19%	5.825%
6	11.128	1396	1401	1404	rBV3	117058	236842	4.26%	0.770%
7	11.833	1517	1521	1525	rBV3	245364	484386	8.71%	1.575%
8	12.398	1612	1617	1622	rBV	525848	910984	16.38%	2.963%
9	12.533	1636	1640	1642	rBV	343466	492846	8.86%	1.603%
10	12.563	1642	1645	1648	rVV2	485449	808180	14.53%	2.628%
11	12.610	1648	1653	1658	rVB	2390081	3668257	65.94%	11.930%
12	12.751	1673	1677	1681	rBV	743374	1290695	23.20%	4.198%
13	13.410	1784	1789	1795	rBV	2701516	4710365	84.67%	15.320%
14	13.733	1840	1844	1847	rBV	1496286	2619452	47.09%	8.519%
15	13.827	1856	1860	1869	rVB	3253252	5563015	100.00%	18.093%

Sum of corrected areas: 30747228

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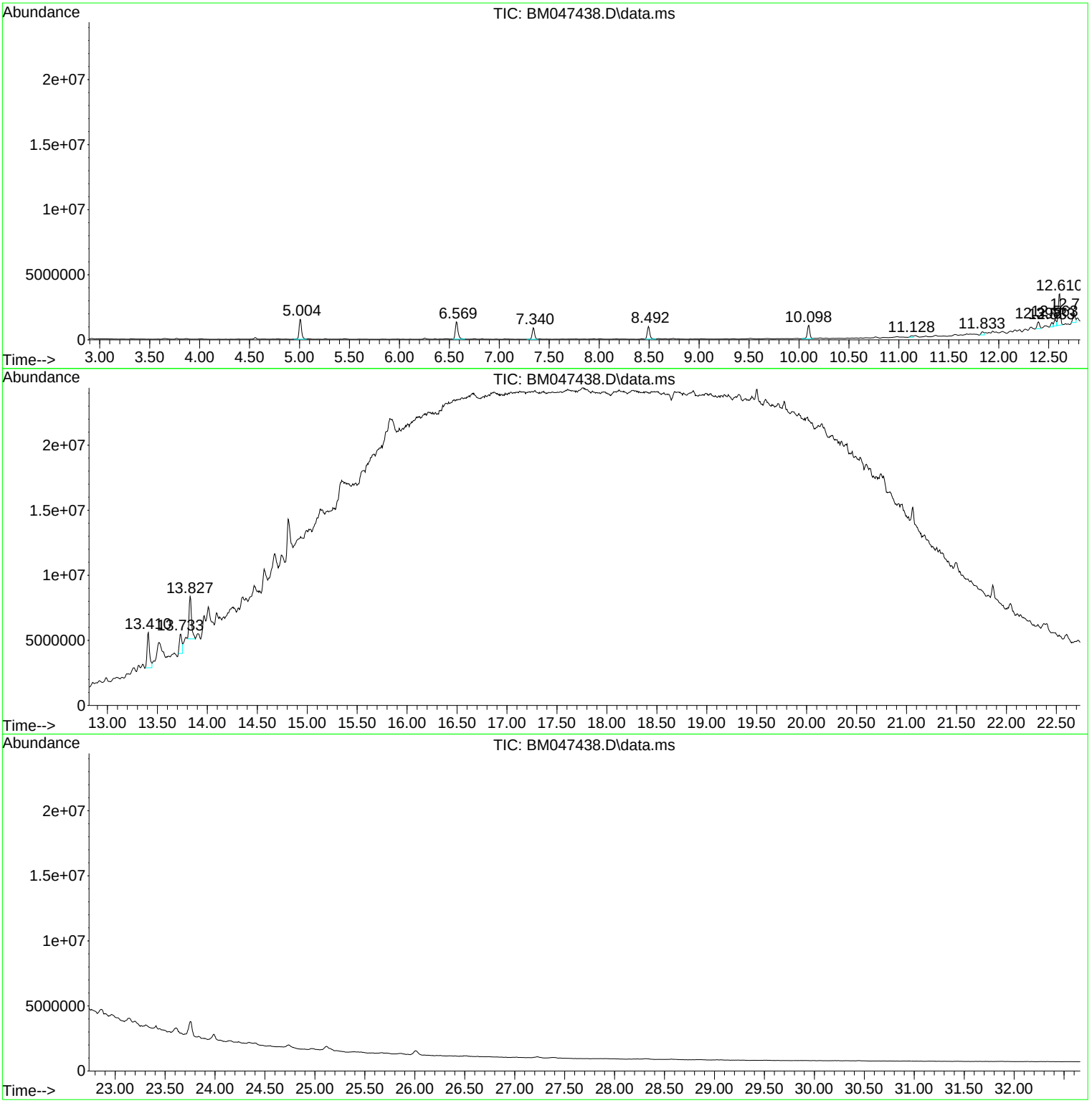
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
Data File : BM047438.D
Acq On : 04 Sep 2024 14:44
Operator : RC/JU
Sample : P3820-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
STONE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

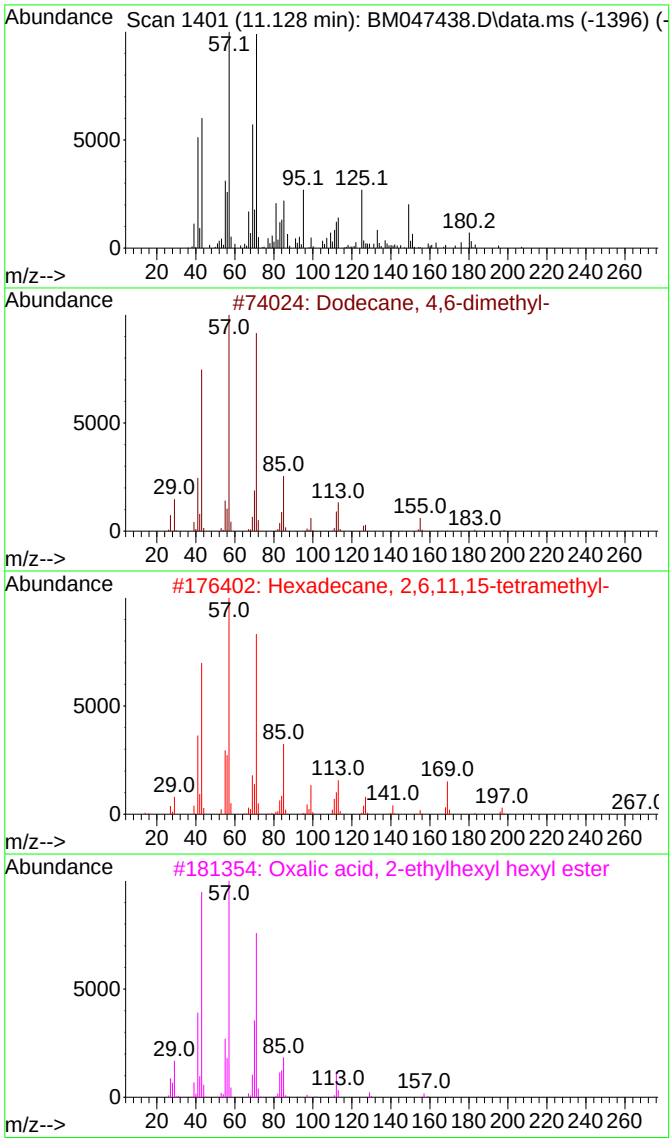
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

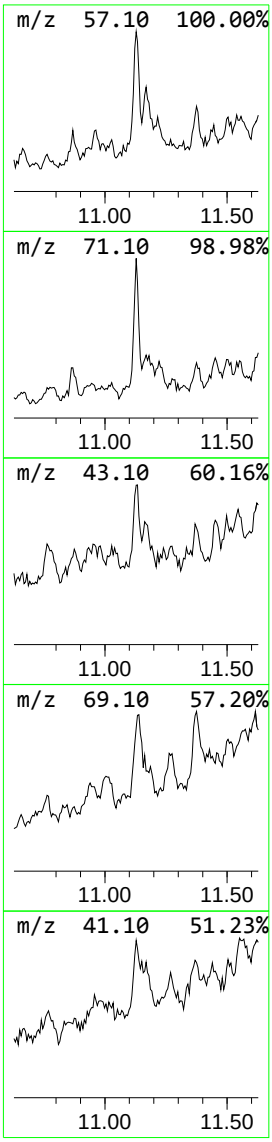
****

Peak Number 1 Dodecane, 4,6-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.128	2.64 ng	236842	Naphthalene-d8	10.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	52
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	50
3	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	50
4	Oxalic acid, octyl propyl ester	244	C13H24O4	1010309-26-1	43
5	Octane, 2,3,6-trimethyl-	156	C11H24	062016-33-5	43





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Data File : BM047438.D
Acq On : 04 Sep 2024 14:44
Operator : RC/JU
Sample : P3820-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

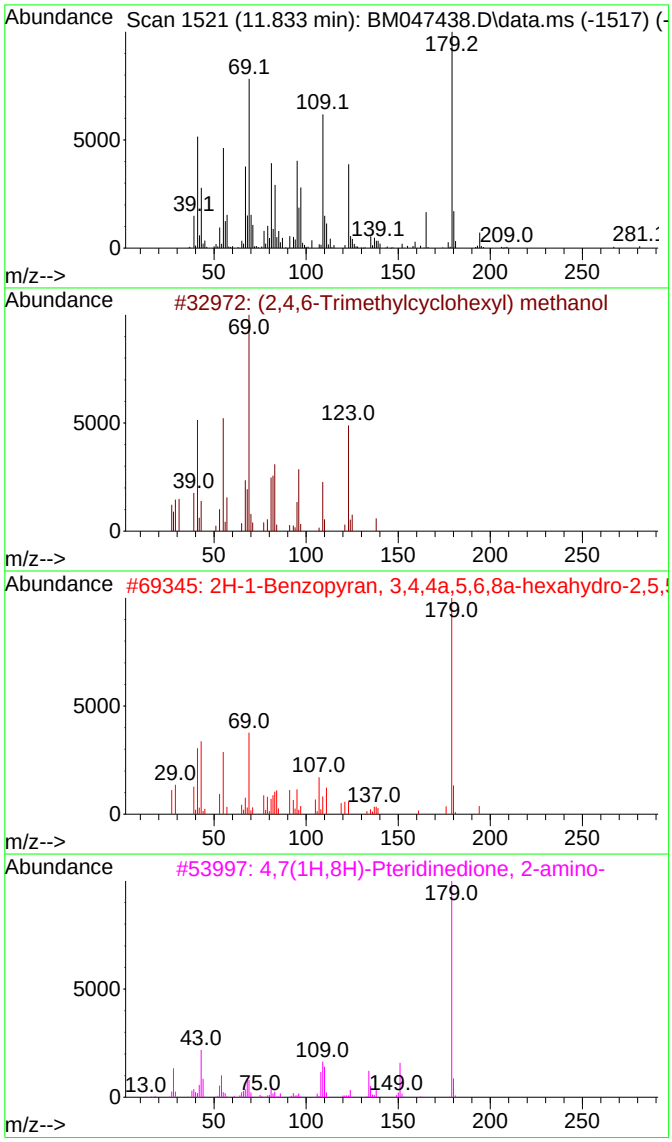
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

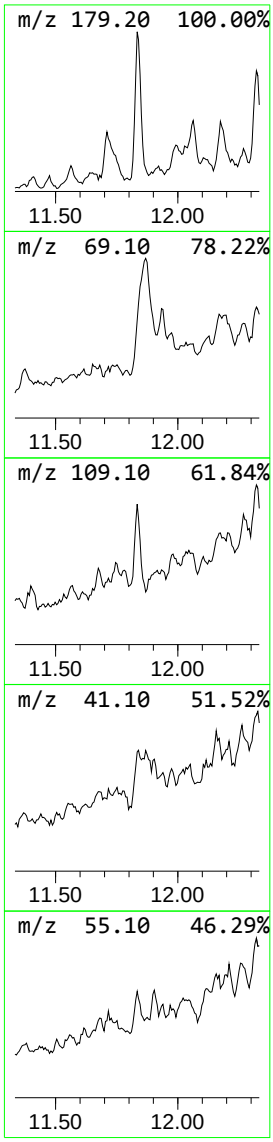
****

Peak Number 2 unknown11.833 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.833	5.41 ng	484386	Naphthalene-d8	10.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2,4,6-Trimethylcyclohexyl) meth...	156	C10H20O	013702-56-2	27
2	2H-1-Benzopyran, 3,4,4a,5,6,8a-h...	194	C13H22O	041678-32-4	22
3	4,7(1H,8H)-Pteridinedione, 2-amino-	179	C6H5N5O2	000529-69-1	18
4	Oxiranecarboxaldehyde, 3-methyl-...	168	C10H16O2	016996-12-6	16
5	2,4,6-Trimethyl-7-oxo-4,7-dihydr...	179	C7H9N5O	025623-78-3	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
Data File : BM047438.D
Acq On : 04 Sep 2024 14:44
Operator : RC/JU
Sample : P3820-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
STONE-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

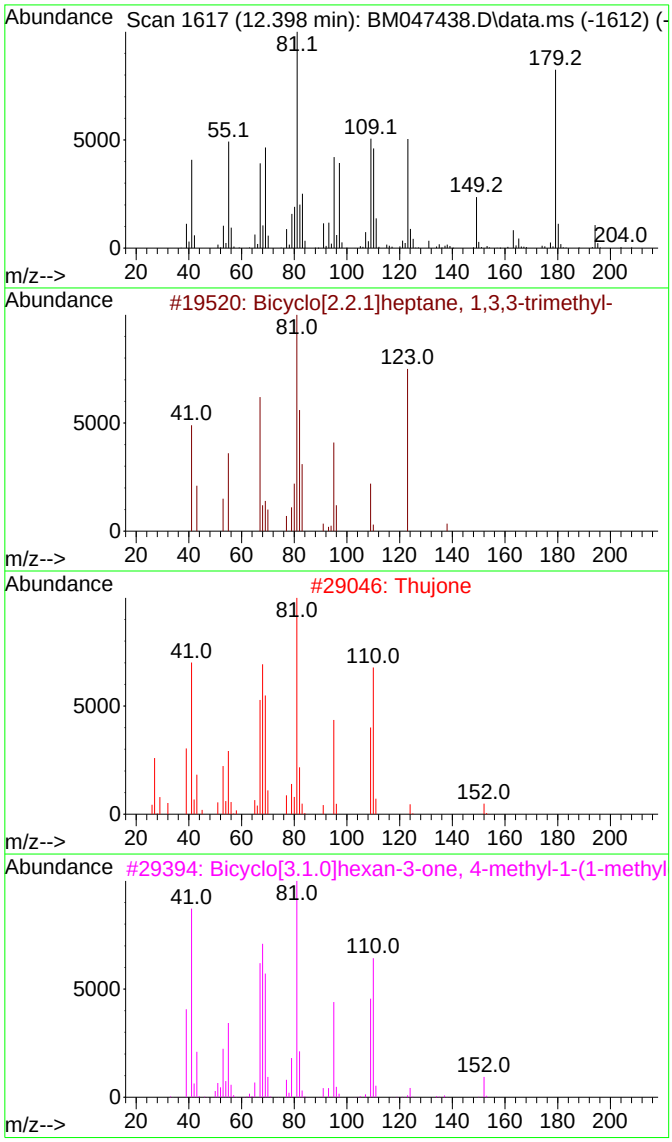
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

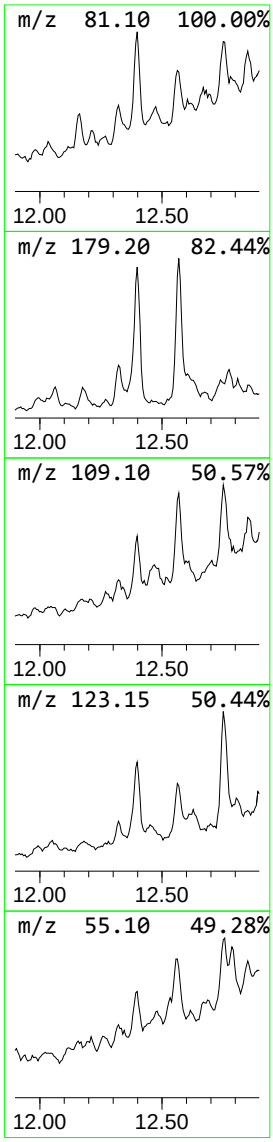
****

Peak Number 3 unknown12.398 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.398	3.28 ng	910984	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	38
2	Thujone	152	C10H16O	000546-80-5	27
3	Bicyclo[3.1.0]hexan-3-one, 4-met...	152	C10H16O	001125-12-8	27
4	Undec-10-ynoic acid	182	C11H18O2	002777-65-3	22
5	1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM090424\
Data File : BM047438.D
Acq On : 04 Sep 2024 14:44
Operator : RC/JU
Sample : P3820-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
STONE-1

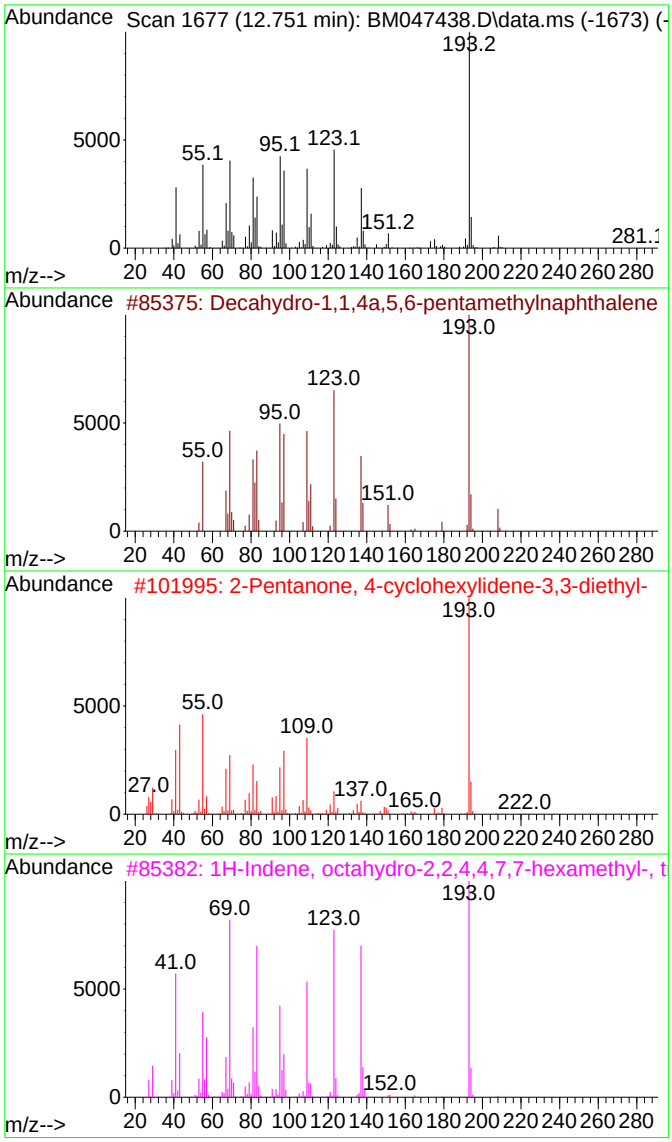
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

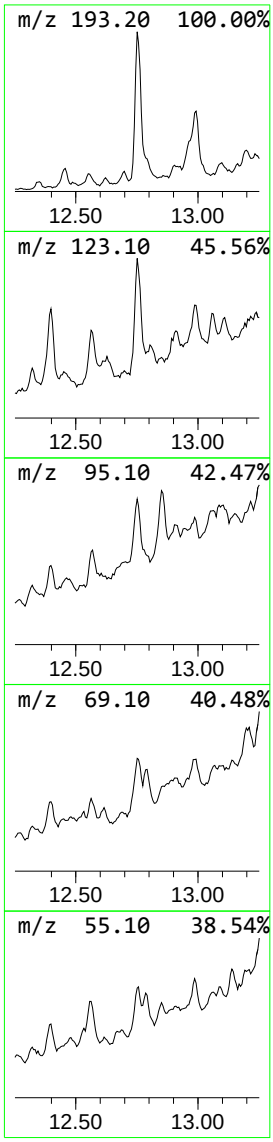
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	4.64 ng	1290700	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	95
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	35
4	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	32
5	2-Anthracenamine	193	C14H11N	000613-13-8	27





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Data File : BM047438.D
Acq On : 04 Sep 2024 14:44
Operator : RC/JU
Sample : P3820-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
STONE-1

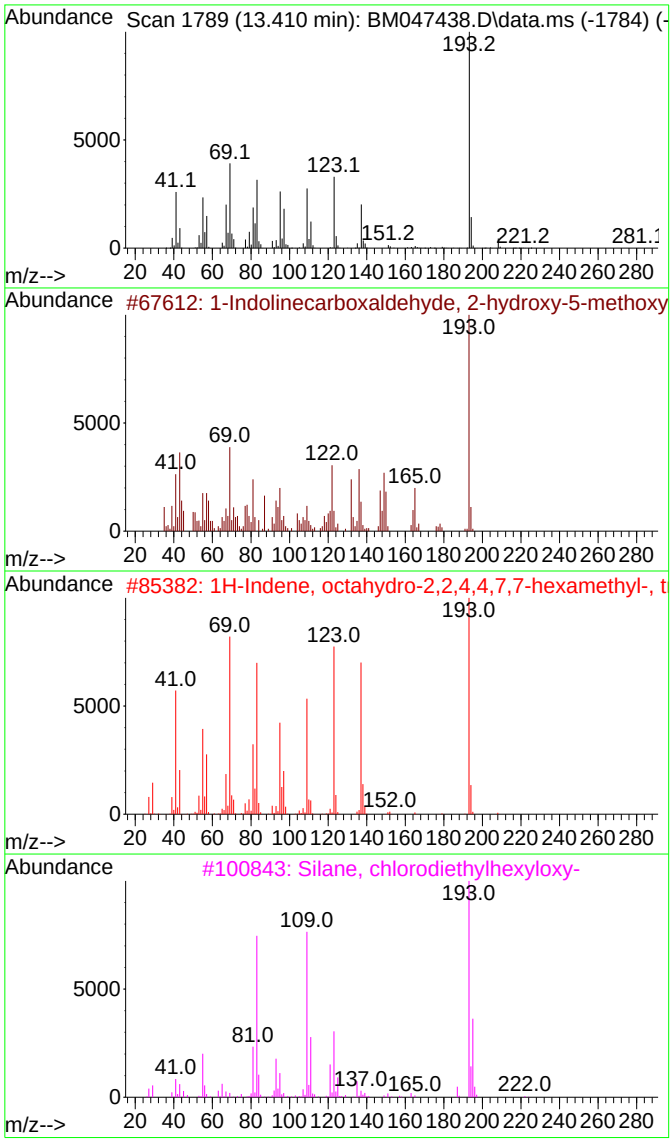
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

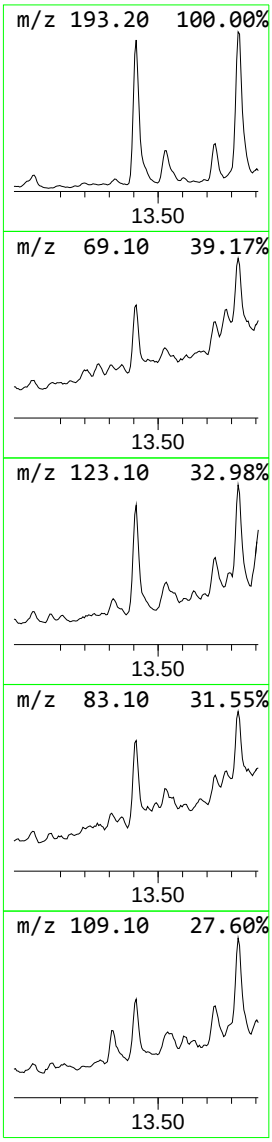
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Indolinecarboxaldehyde, 2... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	16.93 ng	4710370	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11NO3	013303-70-3	53
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	42
3	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	42
4	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	38
5	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	38





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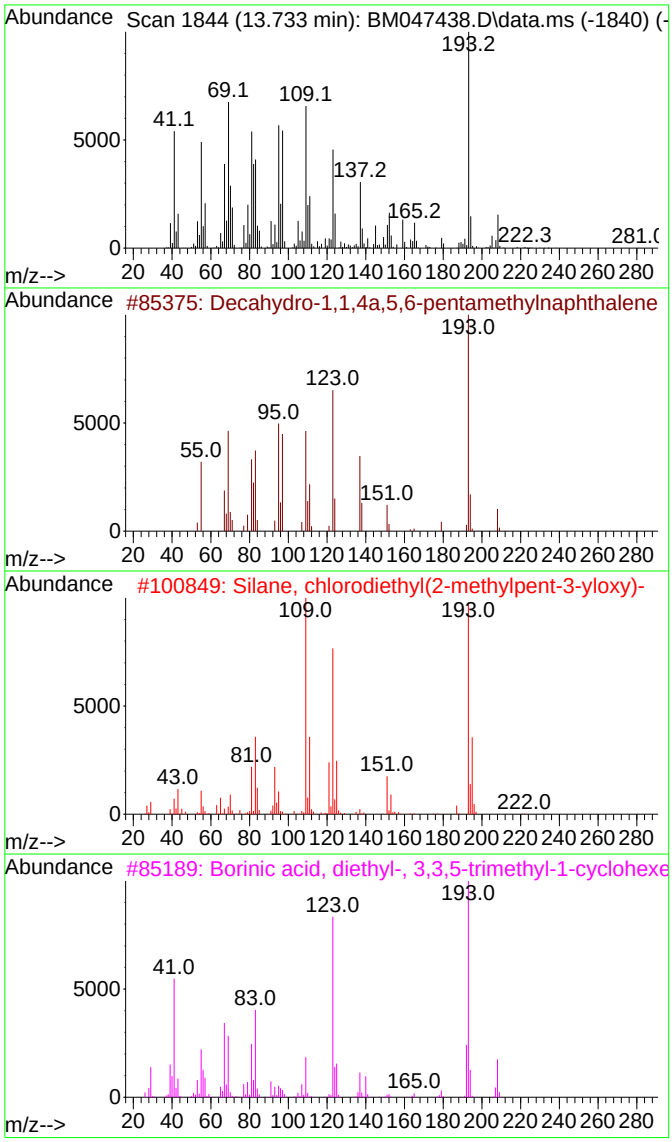
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

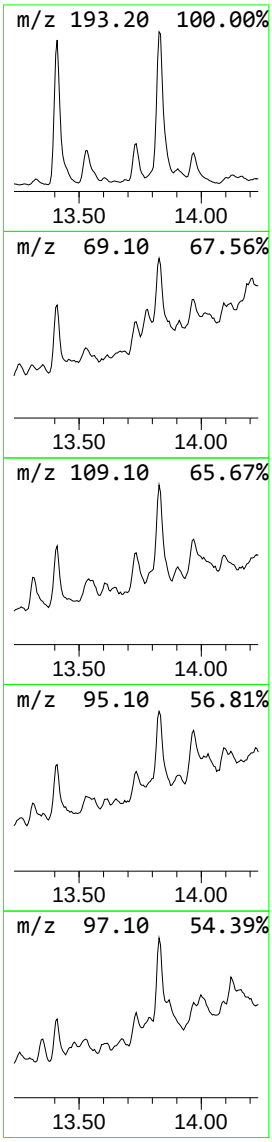
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Silane, chlorodiethyl(2-met... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	9.42 ng	2619450	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	87
2	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	60
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	50
4	Naphthalene, decahydro-1,4a-dime...	208	C15H28	030824-81-8	43
5	2-Anthracenamine	193	C14H11N	000613-13-8	38





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

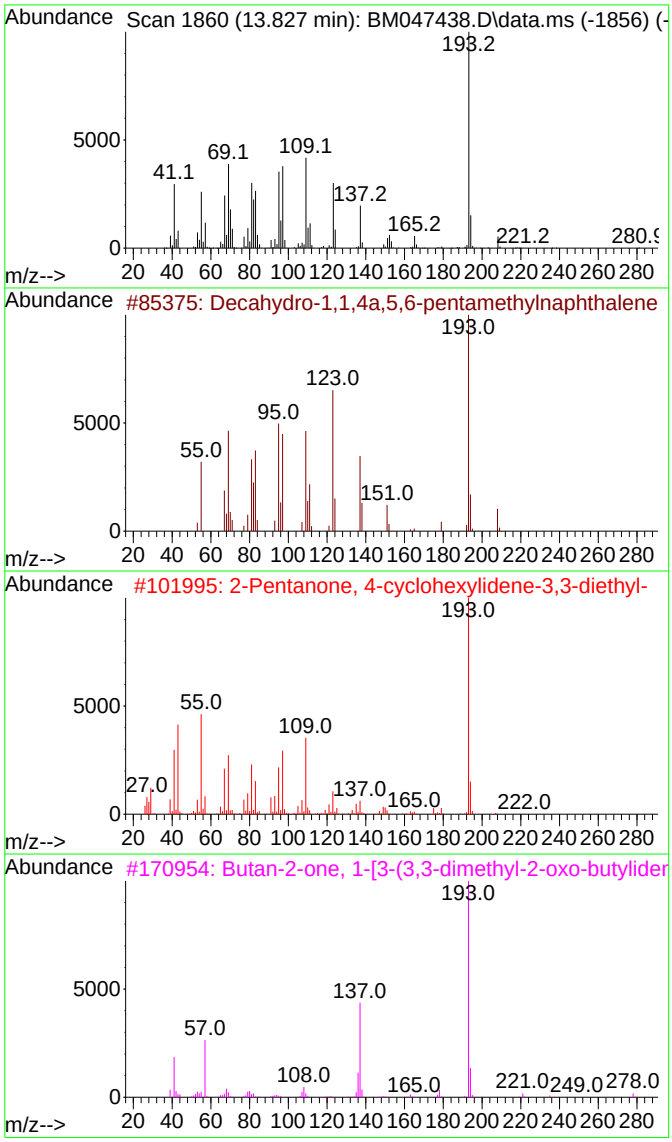
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

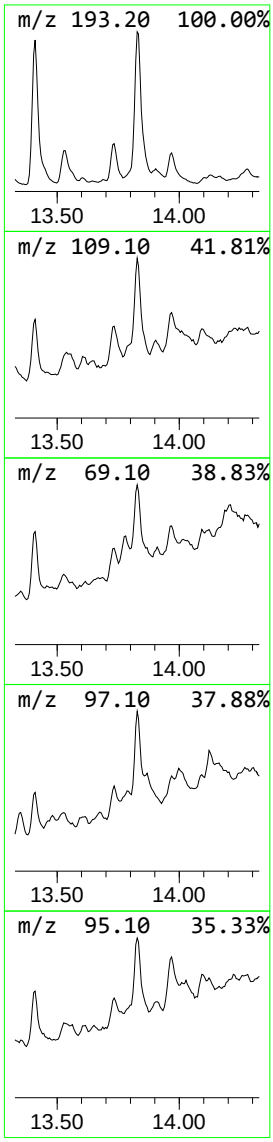
****

Peak Number 7 unknown13.827 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	20.00 ng	5563020	Acenaphthene-d10	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
3	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	35
4	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	32
5	2-Phenylindolizine	193	C14H11N	025379-20-8	30





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Dodecane, 4,6-d...	11.128	2.6	ng	236842	2	10.098	1790990	20.0
unknown11.833	11.833	5.4	ng	484386	2	10.098	1790990	20.0
unknown12.398	12.398	3.3	ng	910984	3	14.010	5563020	20.0
Decahydro-1,1,4...	12.751	4.6	ng	1290700	3	14.010	5563020	20.0
1-Indolinecarbo...	13.410	16.9	ng	4710370	3	14.010	5563020	20.0
Silane, chlorod...	13.733	9.4	ng	2619450	3	14.010	5563020	20.0
unknown13.827	13.827	20.0	ng	5563020	3	14.010	5563020	20.0