LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005540.D
Acq On : 14 May 2021 02:46
Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-27051

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005540.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.293	368	375	388	rBV	64850	116490	14.22%	2.137%
2	6.911	643	650	658	rBV	51542	110057	13.44%	2.019%
3	7.687	774	782	790	rBV	107914	170906	20.87%	3.135%
4	8.858	975	981	988	rBV2	45543	79574	9.72%	1.460%
5	10.216	1199	1212	1228	rBV	48206	132702	16.20%	2.435%
6	10.481	1247	1257	1264	rVB	133582	232070	28.34%	4.258%
7	10.681	1282	1291	1298	rBV2	65110	128562	15.70%	2.359%
8	12.963	1668	1679	1684	rBV	181928	350694	42.82%	6.434%
9	13.110	1699	1704	1707	rBV3	69824	114878	14.03%	2.108%
10	13.687	1799	1802	1808	rVB	82790	119411	14.58%	2.191%
11	13.751	1809	1813	1818	rVB	148601	199347	24.34%	3.657%
12	14.069	1864	1867	1871	rBV4	72788	114831	14.02%	2.107%
13	14.163	1879	1883	1888	rVB	250795	305205	37.27%	5.599%
14	14.298	1902	1906	1909	rBV3	152936	269619	32.92%	4.946%
15	14.345	1910	1914	1922	rVB2	302498	565014	68.99%	10.366%
16	14.669	1966	1969	1972	rBV2	90009	126773	15.48%	2.326%
17	15.128	2043	2047	2052	rBV2	432073	637542	77.85%	11.696%
18	21.204	3076	3080	3085	rVB	371238	461482	56.35%	8.466%
19	21.839	3184	3188	3192	rVB2	726150	818982	100.00%	15.025%
20	23.516	3468	3473	3479	rVB	214999	396687	48.44%	7.278%

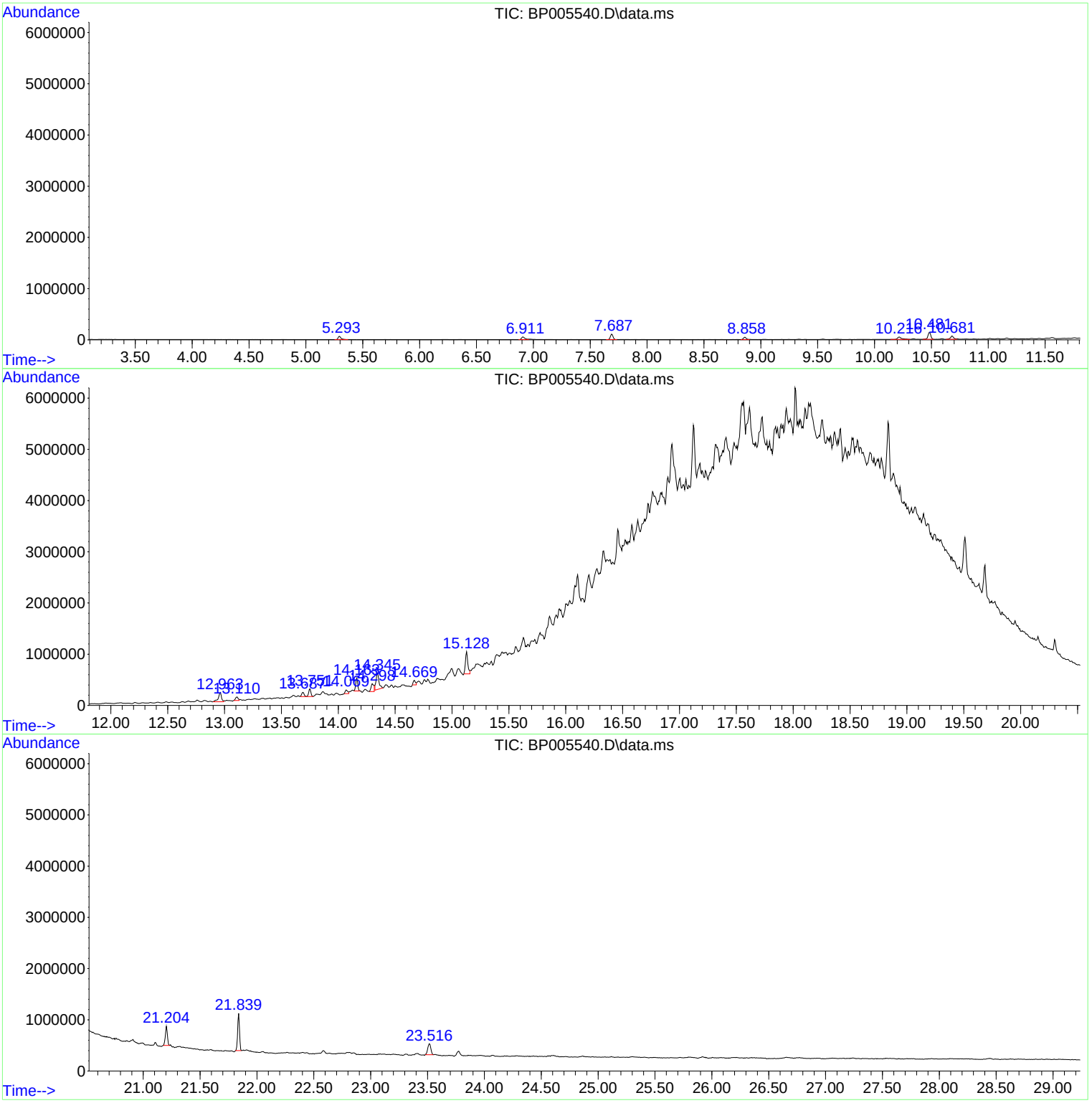
Sum of corrected areas: 5450826

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005540.D
Acq On : 14 May 2021 02:46
Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-27051

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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 : BP005540.D
Acq On : 14 May 2021 02:46
Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-27051

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

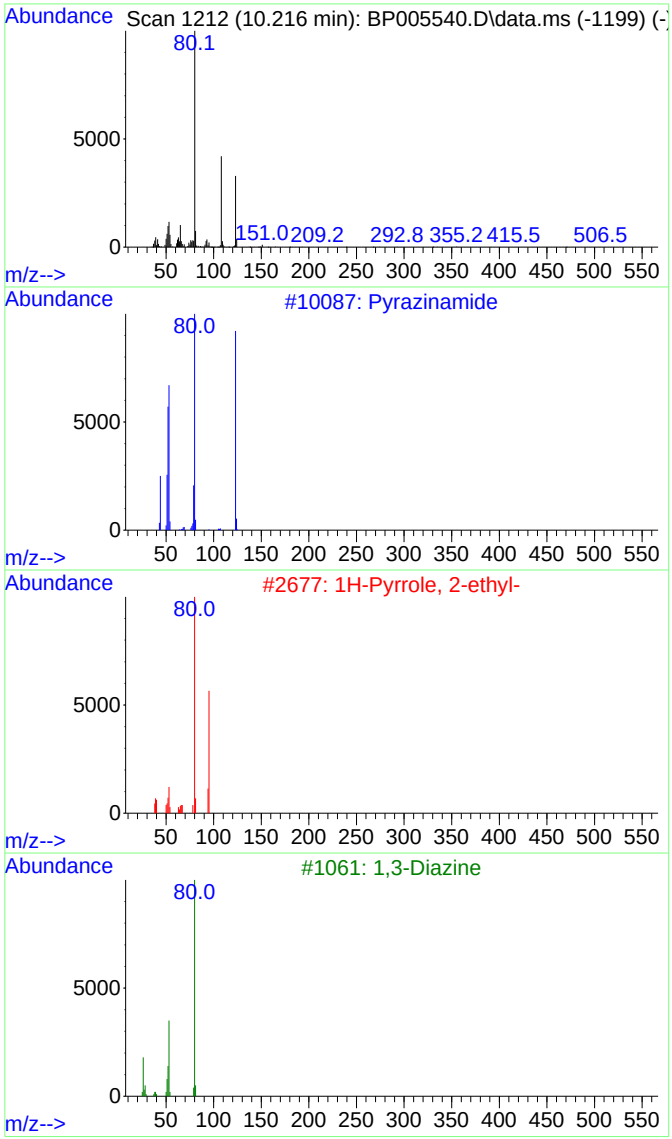
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

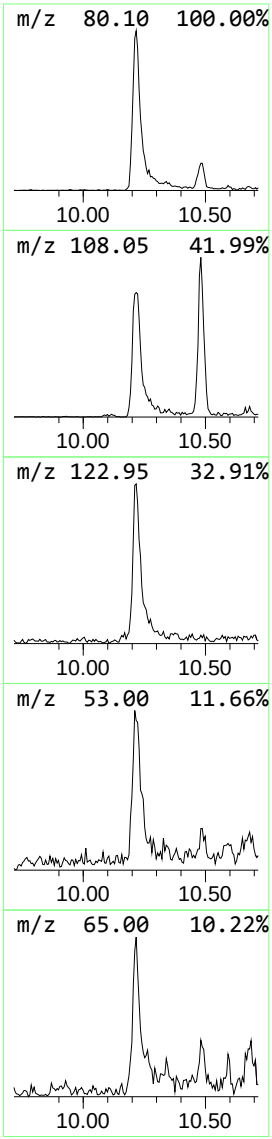
****

Peak Number 1 Pyrazinamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.216	11.44 ng	132702	Naphthalene-d8	10.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazinamide	123	C5H5N3O	000098-96-4	72
2	1H-Pyrrole, 2-ethyl-	95	C6H9N	001551-06-0	64
3	1,3-Diazine	80	C4H4N2	000289-95-2	59
4	3-Pyridinemethanamine	108	C6H8N2	003731-52-0	56
5	1-Penten-3-yne, 2-methyl-	80	C6H8	000926-55-6	50





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Data File : BP005540.D
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Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-27051

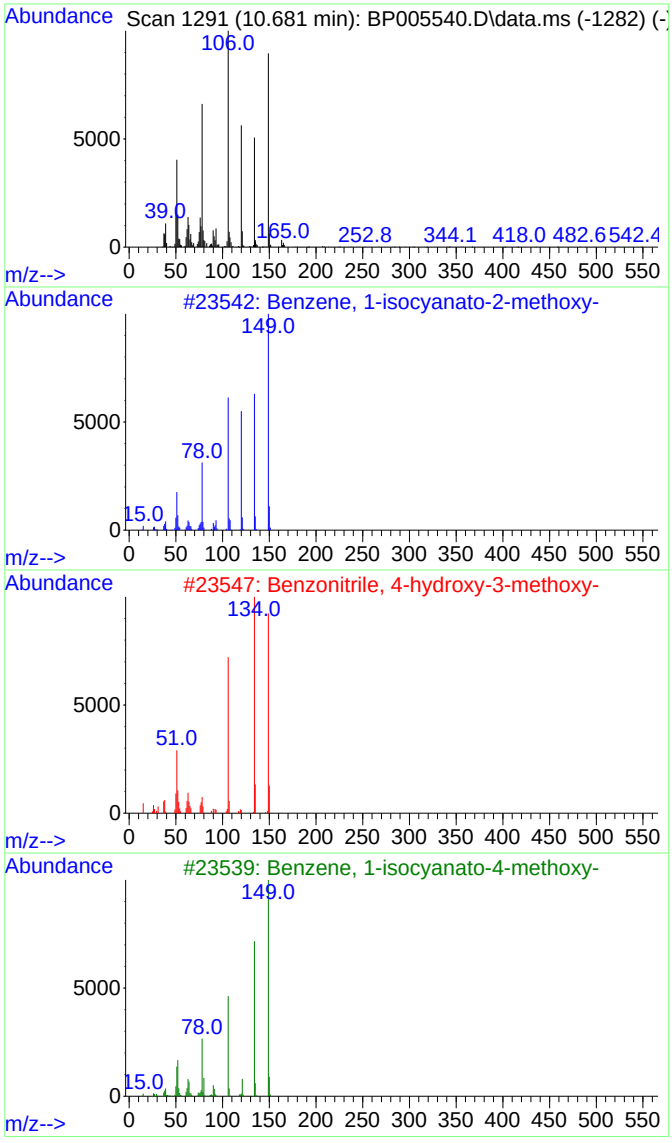
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

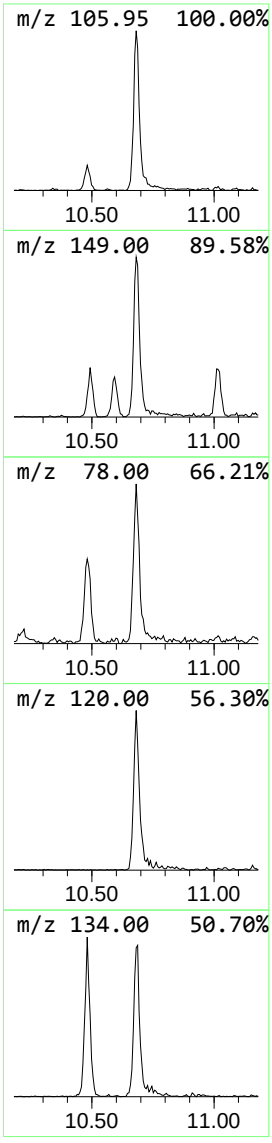
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1-isocyanato-2-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.681	11.08 ng	128562	Naphthalene-d8	10.481

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	94
2	Benzonitrile, 4-hydroxy-3-methoxy-	149	C8H7NO2	004421-08-3	49
3	Benzene, 1-isocyanato-4-methoxy-	149	C8H7NO2	005416-93-3	43
4	2-(Methoxycarbonyl)phenyl nicoti...	257	C14H11NO4	023723-12-8	38
5	o-Nitrobenzaldehyde isonicotinhy...	270	C13H10N4O3	005505-71-5	35





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Data File : BP005540.D
Acq On : 14 May 2021 02:46
Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-27051

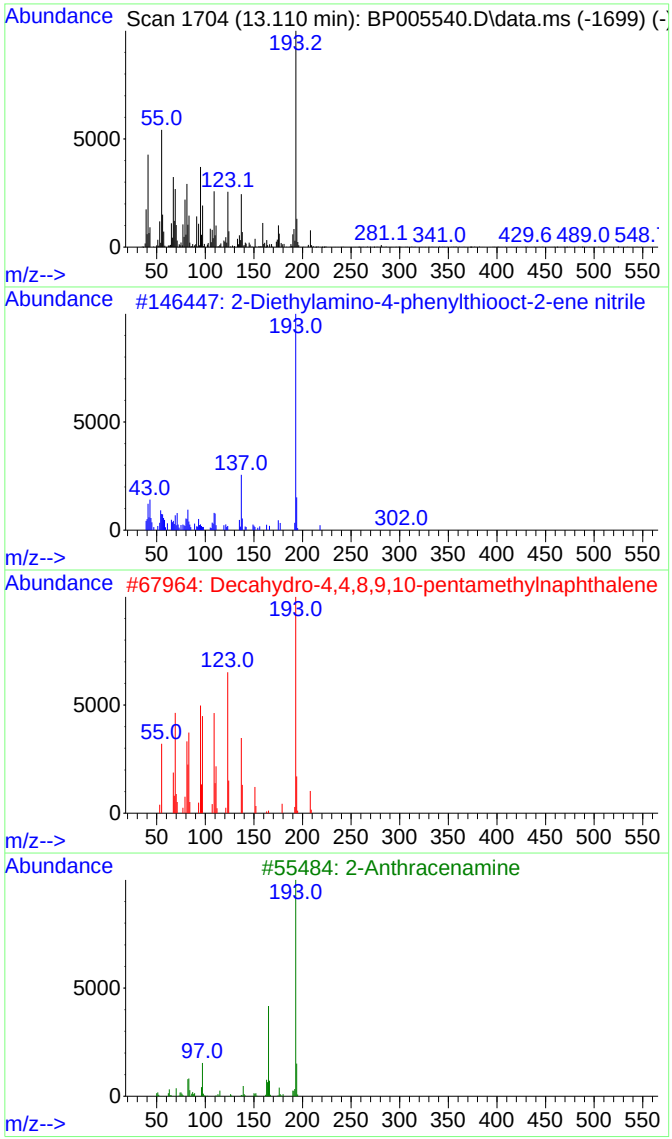
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

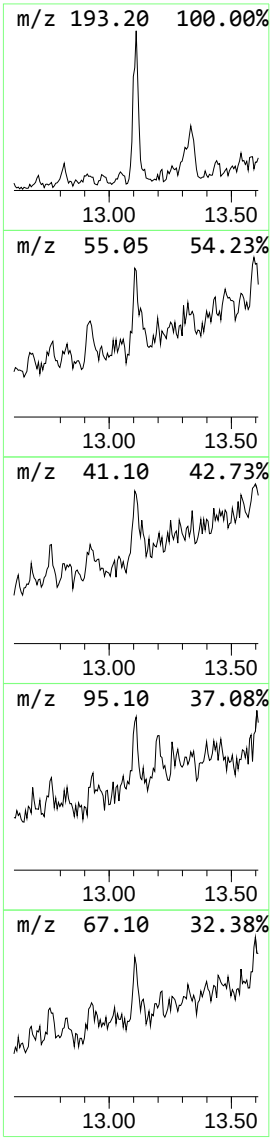
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Diethylamino-4-phenylthio... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.110	4.07 ng	114878	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	55
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	50
3	2-Anthracenamine	193	C14H11N	000613-13-8	38
4	Methanone, (cyclohexyl)(2,5-diet...	276	C17H24O3	076185-89-2	38
5	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	38





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Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-27051

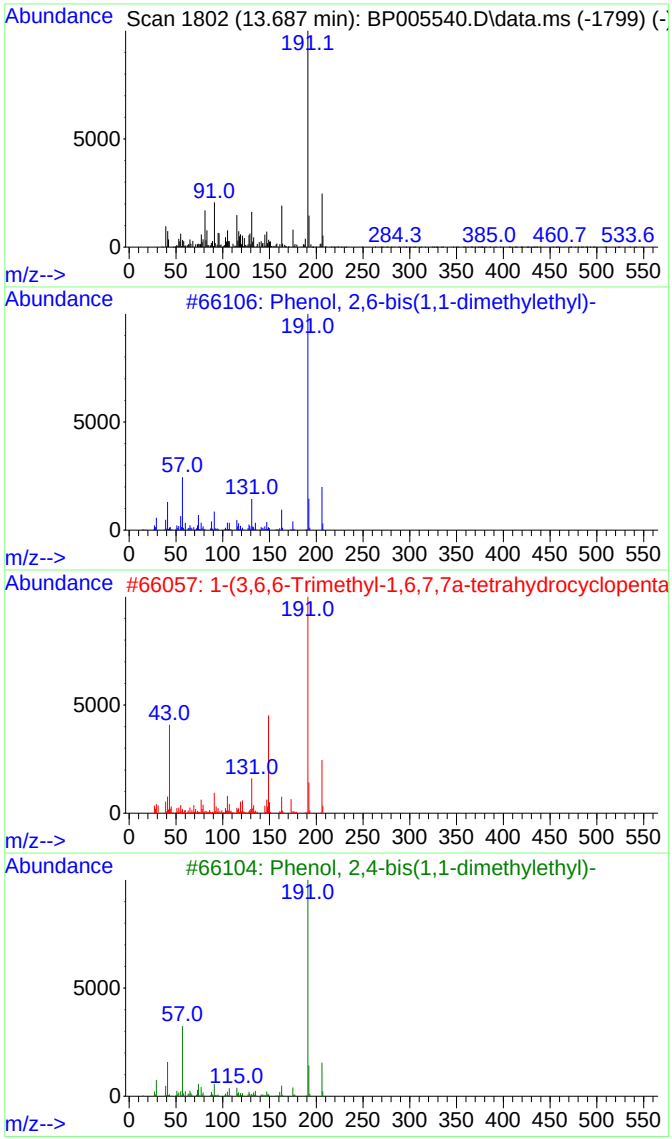
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

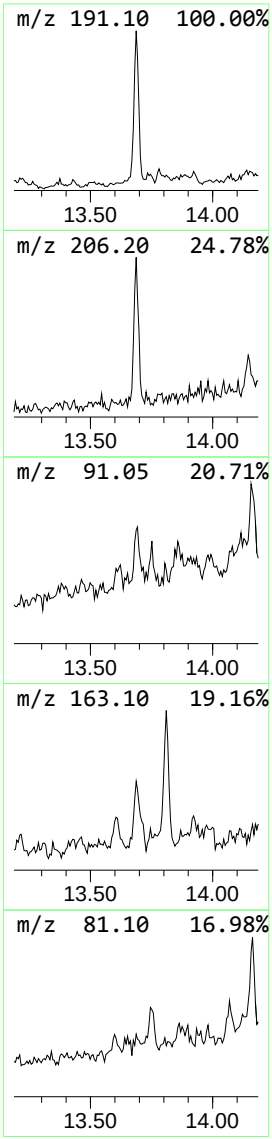
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.687	4.23 ng	119411	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	87
2	1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	81
3	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	76
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	76
5	2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005540.D
Acq On : 14 May 2021 02:46
Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-27051

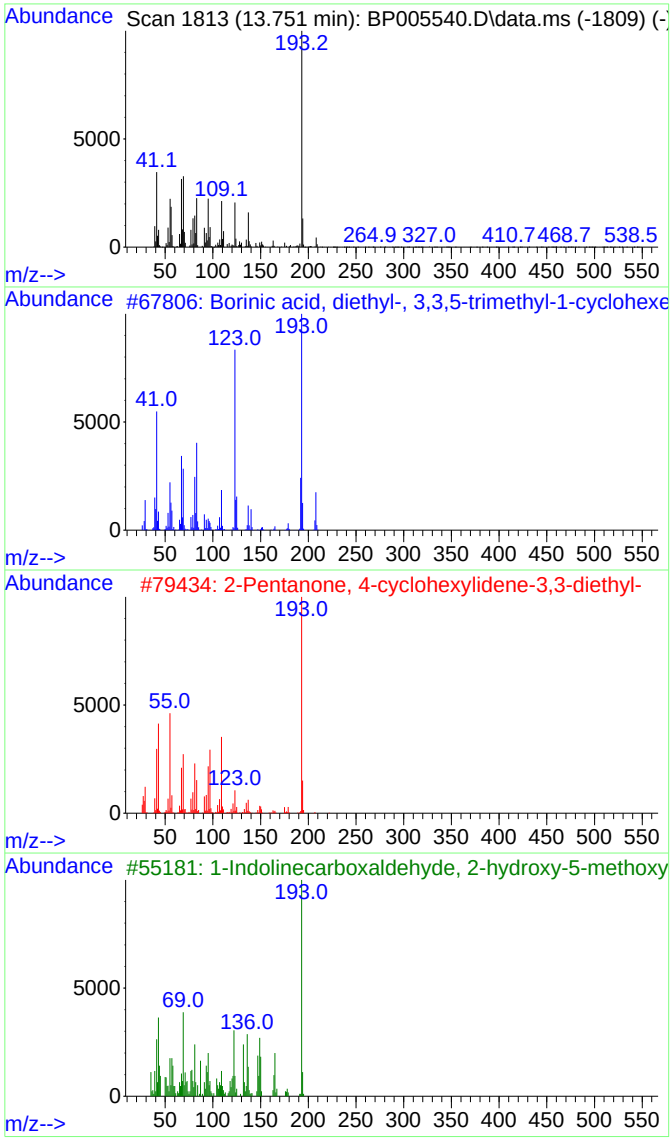
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

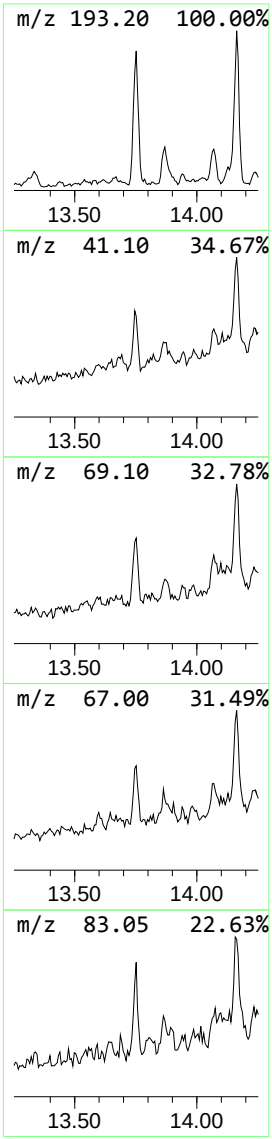
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Borinic acid, diethyl-, 3,3... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	7.06 ng	199347	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	59
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	50
3	1-Indolinecarboxaldehyde, 2-hydr...	193	C10H11NO3	013303-70-3	50
4	9-Vinylcarbazole	193	C14H11N	001484-13-5	35
5	Iminostilbene	193	C14H11N	000256-96-2	35





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Data File : BP005540.D
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Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CHRT-27051

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

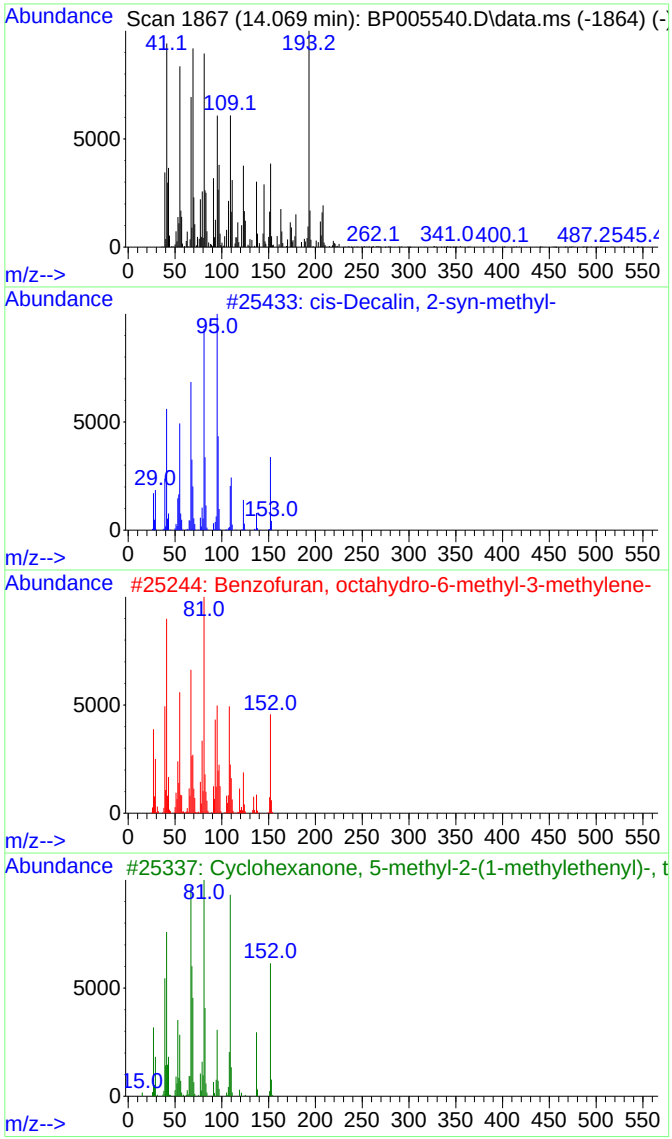
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

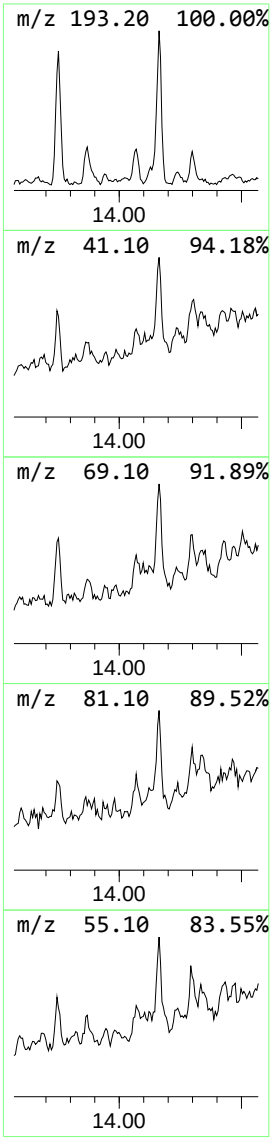
****

Peak Number 6 unknown14.069 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.069	4.06 ng	114831	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	38
2	Benzofuran, octahydro-6-methyl-3...	152	C10H16O	077954-13-3	27
3	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	029606-79-9	27
4	Spiro[4.5]decan-2-one	152	C10H16O	003643-16-1	25
5	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	25





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Misc :
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Instrument :
BNA_P
ClientSampleId :
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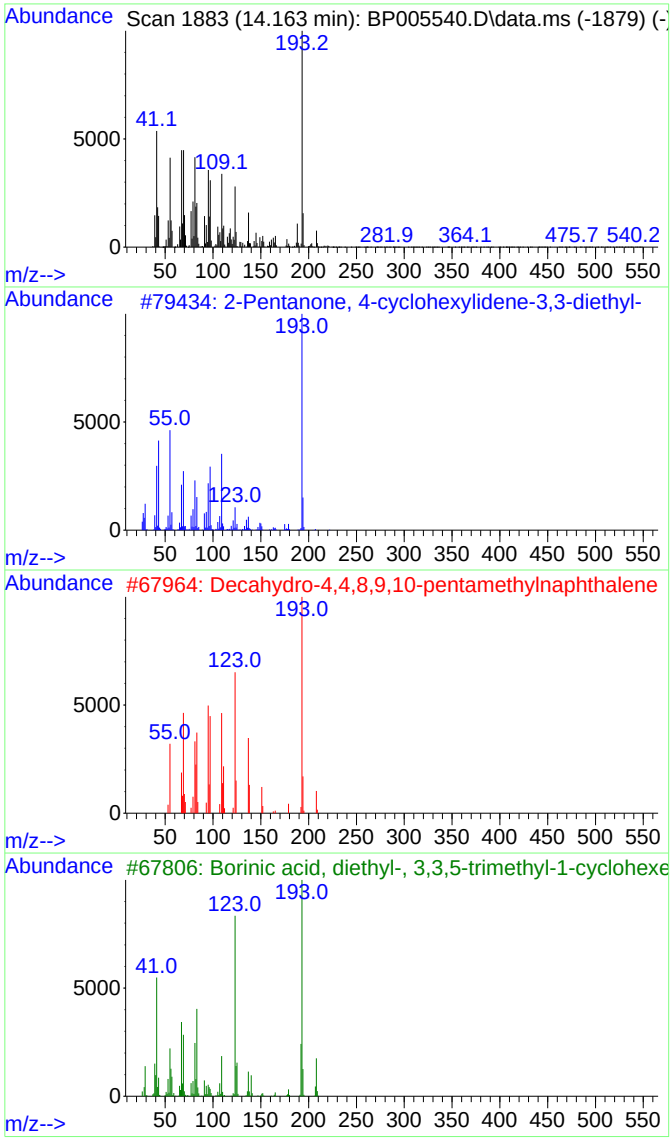
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

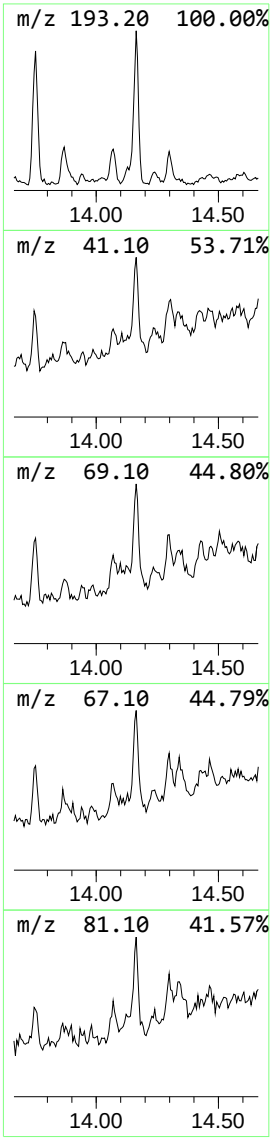
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Pentanone, 4-cyclohexylid... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	10.80 ng	305205	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	59
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	53
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	40
4	3-Phenylindole	193	C14H11N	001504-16-1	30
5	6-Methylphenanthridine	193	C14H11N	003955-65-5	27





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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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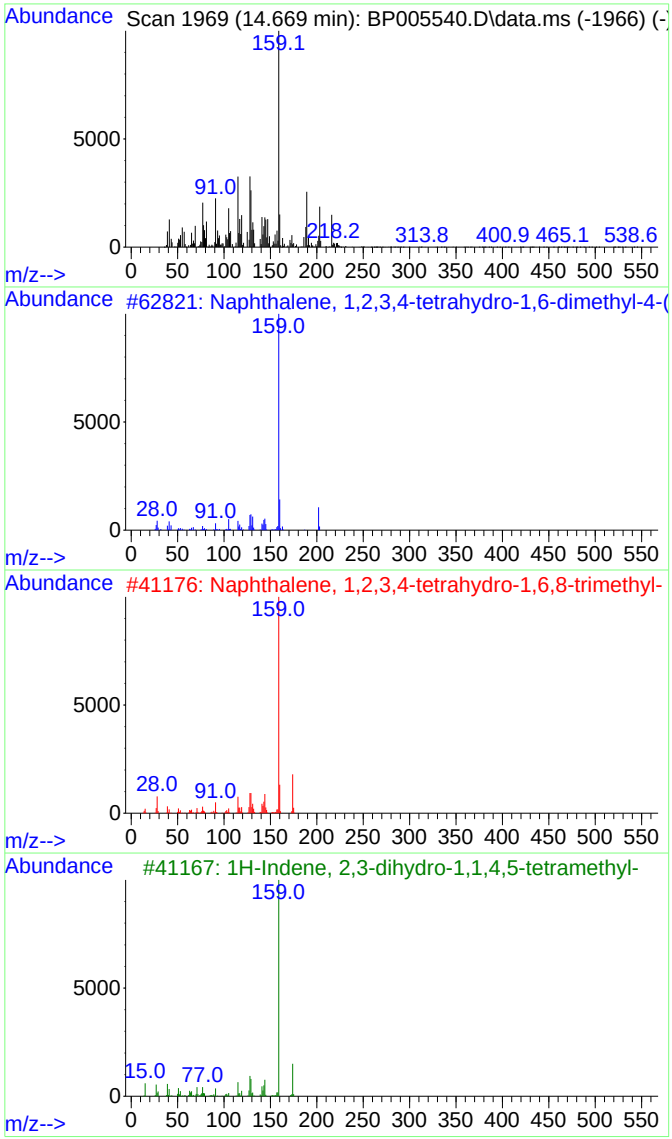
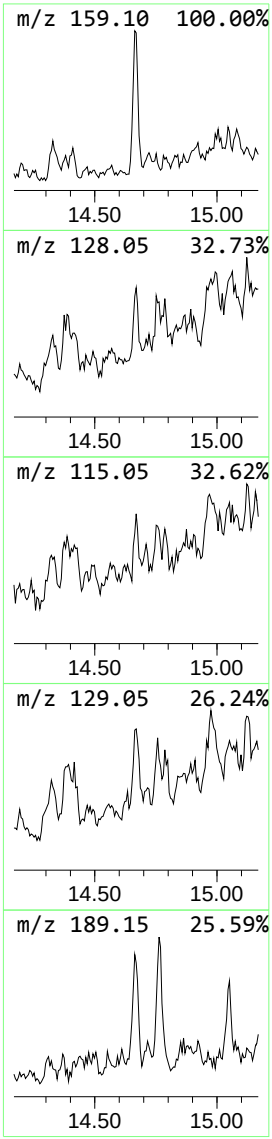
****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.669	4.49 ng	126773	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	83
2	Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	64
3	1H-Indene, 2,3-dihydro-1,1,4,5-t...	174	C13H18	016204-57-2	60
4	1H-Indene, 2,3-dihydro-1,1,4,6-t...	174	C13H18	000941-60-6	60
5	Acetamide, 2-(2-ethyl-1-benzimid...	203	C11H13N3O	054980-94-8	45





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TIC Library : C:\DATABASE\NIST11.L
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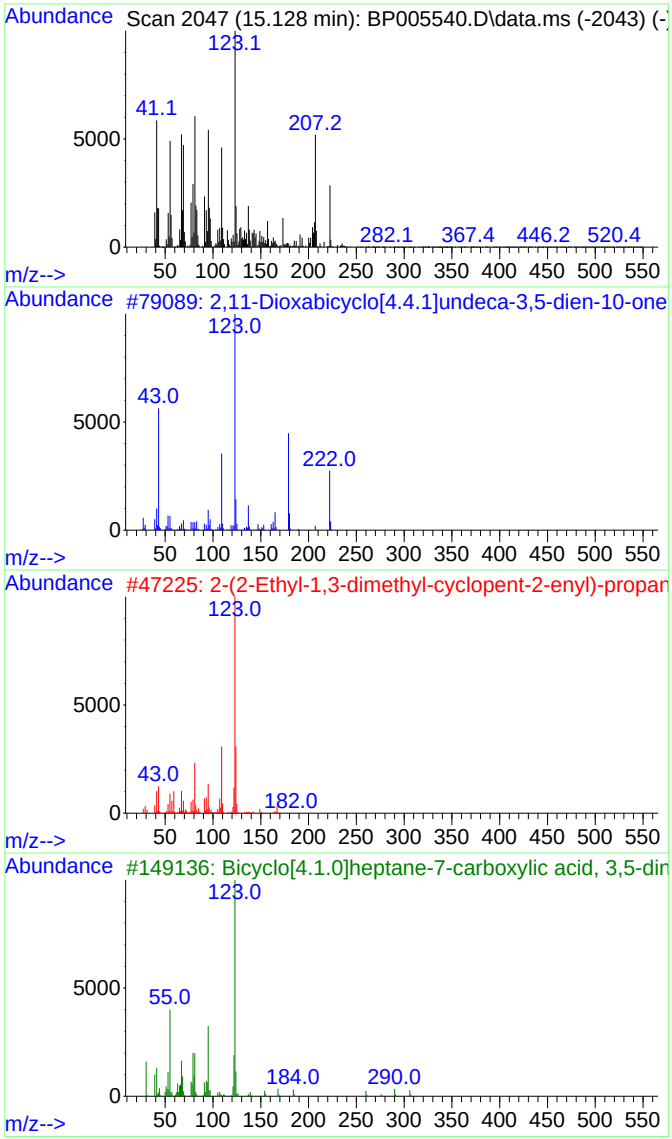
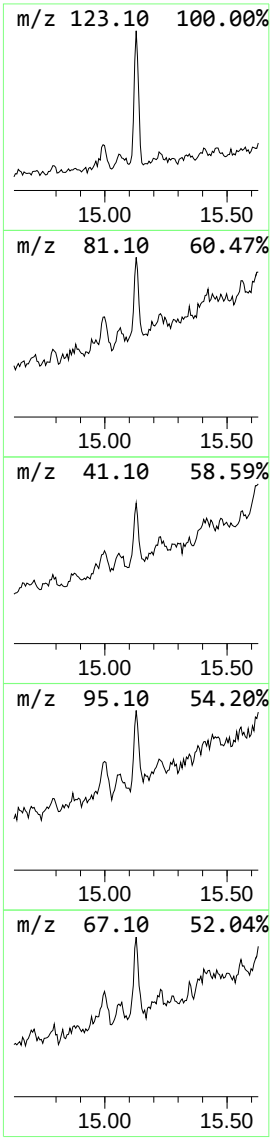
Peak Number 9 unknown15.128 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.128	22.57 ng	637542	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...	222	C13H18O3	070412-52-1	43
2	2-(2-Ethyl-1,3-dimethyl-cyclopen...	182	C12H22O	1000186-82-4	38
3	Bicyclo[4.1.0]heptane-7-carboxyl...	306	C14H14N2O6	1000311-95-8	38
4	Magnesium, bis(2,4-pentanedionat...	222	C10H14MgO4	014024-56-7	38
5	2-Cyclohexen-1-one, 5-bromo-4,4-...	202	C8H11BrO	1000327-26-6	35





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Acq On : 14 May 2021 02:46
Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CHRT-27051

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
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TIC Integration Parameters: LSCINT.P

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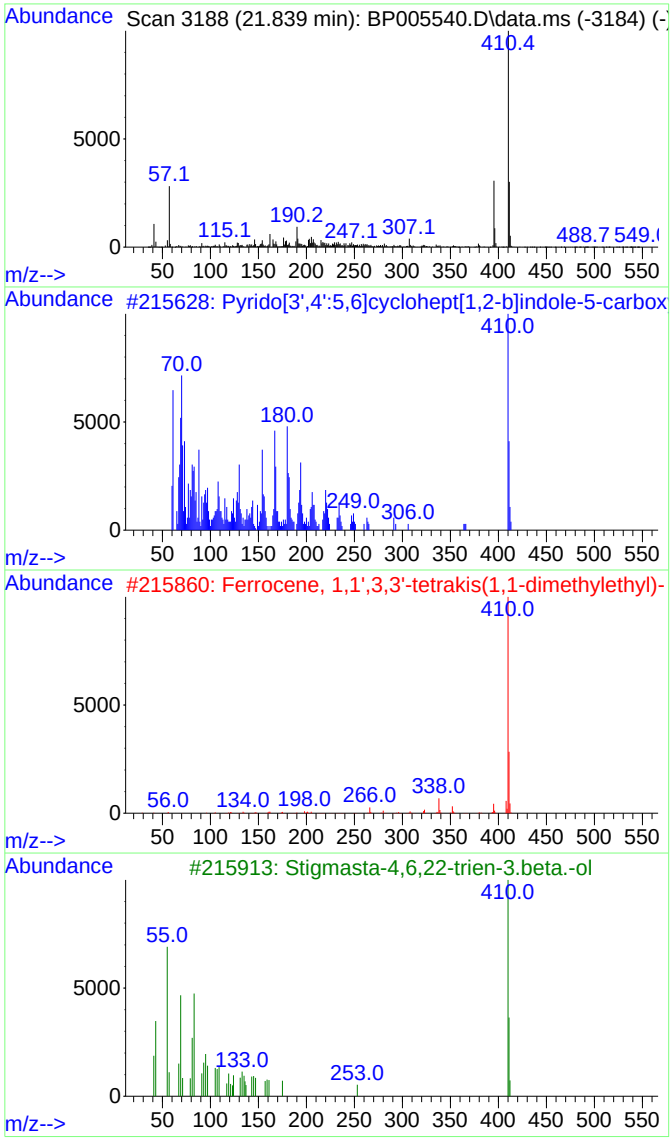
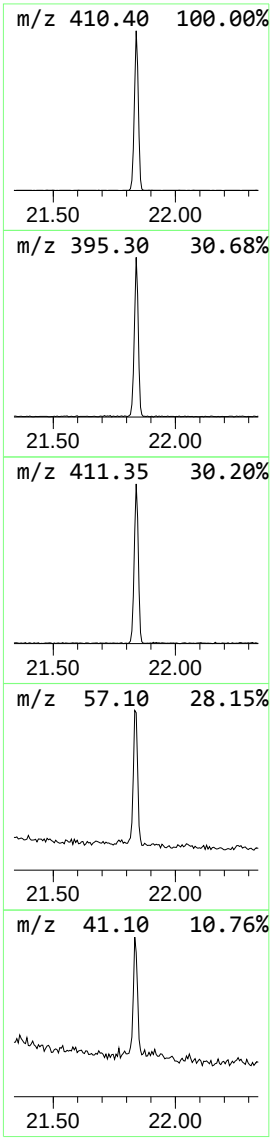
Peak Number 10 Pyrido[3',4':5,6]cyclohept[... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.839	35.49 ng	818982	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrido[3',4':5,6]cyclohept[1,2-b...	410	C23H26N2O5	003368-89-6	98
2	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	70
3	Stigmasta-4,6,22-trien-3.beta.-ol	410	C29H46O	096737-58-5	52
4	3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	45
5	.DELTA.9-THC TFA	410	C23H29F3O3	086702-79-6	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051321\
Data File : BP005540.D
Acq On : 14 May 2021 02:46
Operator : CG/JU
Sample : M2372-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CHRT-27051

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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
Pyrazinamide	10.216	11.4	ng	132702	2	10.481	232070	20.0
Benzene, 1-isoc...	10.681	11.1	ng	128562	2	10.481	232070	20.0
2-Diethylamino-...	13.110	4.1	ng	114878	3	14.345	565014	20.0
Phenol, 2,6-bis...	13.687	4.2	ng	119411	3	14.345	565014	20.0
Borinic acid, d...	13.751	7.1	ng	199347	3	14.345	565014	20.0
unknown14.069	14.069	4.1	ng	114831	3	14.345	565014	20.0
2-Pentanone, 4-...	14.163	10.8	ng	305205	3	14.345	565014	20.0
Naphthalene, 1,...	14.669	4.5	ng	126773	3	14.345	565014	20.0
unknown15.128	15.128	22.6	ng	637542	3	14.345	565014	20.0
Pyrido[3',4':5,...	21.839	35.5	ng	818982	5	21.204	461482	20.0