LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120321\
Data File : BP008221.D
Acq On : 04 Dec 2021 00:13
Operator : CG/JU
Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

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-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008221.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.222	36	40	52	rVB	59857	94636	5.74%	0.738%
2	4.922	323	329	338	rBV	33502	52135	3.16%	0.407%
3	5.387	402	408	424	rVB	265946	420459	25.49%	3.280%
4	6.981	666	679	693	rBV	235122	435457	26.40%	3.397%
5	7.793	809	817	826	rBV	412291	655552	39.75%	5.113%
6	8.951	1007	1014	1025	rBV	154702	276630	16.77%	2.158%
7	10.593	1284	1293	1308	rBV	536067	932206	56.52%	7.271%
8	13.063	1704	1713	1723	rBV	417530	703000	42.62%	5.483%
9	13.222	1736	1740	1745	rBV2	58588	88491	5.37%	0.690%
10	13.763	1829	1832	1837	rBV3	39142	59063	3.58%	0.461%
11	13.863	1844	1849	1856	rBV	314857	457009	27.71%	3.565%
12	13.981	1865	1869	1877	rVB3	74734	139035	8.43%	1.084%
13	14.181	1898	1903	1909	rBV6	125503	267053	16.19%	2.083%
14	14.275	1915	1919	1925	rVB	371769	532844	32.31%	4.156%
15	14.345	1927	1931	1937	rBV3	78764	152509	9.25%	1.190%
16	14.410	1937	1942	1943	rBV	160015	215009	13.04%	1.677%
17	14.445	1943	1948	1955	rVV	852691	1323652	80.25%	10.325%
18	14.534	1959	1963	1969	rVV2	81481	139439	8.45%	1.088%
19	14.769	1999	2003	2007	rBV2	62956	122240	7.41%	0.953%
20	14.975	2035	2038	2040	rBV2	57949	75591	4.58%	0.590%
21	15.075	2052	2055	2057	rBV4	66267	92377	5.60%	0.721%
22	15.104	2057	2060	2065	rVB3	119117	177808	10.78%	1.387%
23	15.163	2066	2070	2076	rBV4	127025	211532	12.83%	1.650%
24	15.233	2078	2082	2089	rVB2	302297	468320	28.39%	3.653%
25	15.945	2198	2203	2208	rBV	334293	563737	34.18%	4.397%
26	16.198	2239	2246	2251	rBV2	349124	729025	44.20%	5.686%
27	17.028	2384	2387	2397	rVB	388871	579891	35.16%	4.523%
28	17.210	2413	2418	2422	rBV	1100693	1649339	100.00%	12.865%
29	19.780	2852	2855	2865	rVB	928745	1206317	73.14%	9.409%

Sum of corrected areas: 12820356

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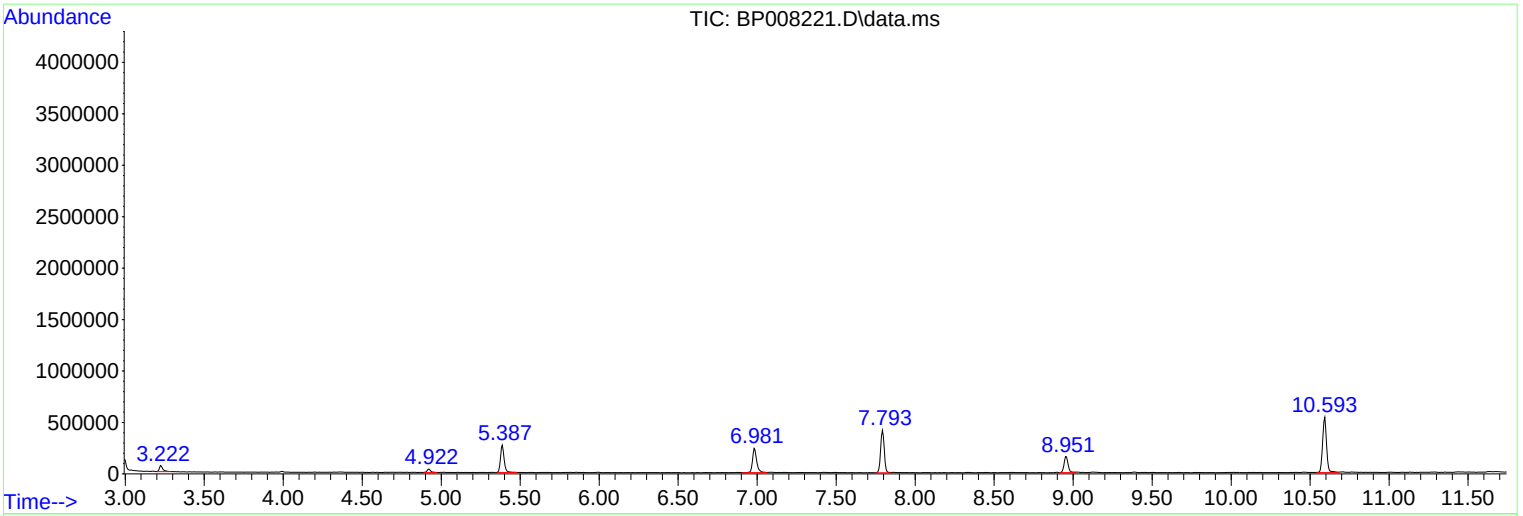
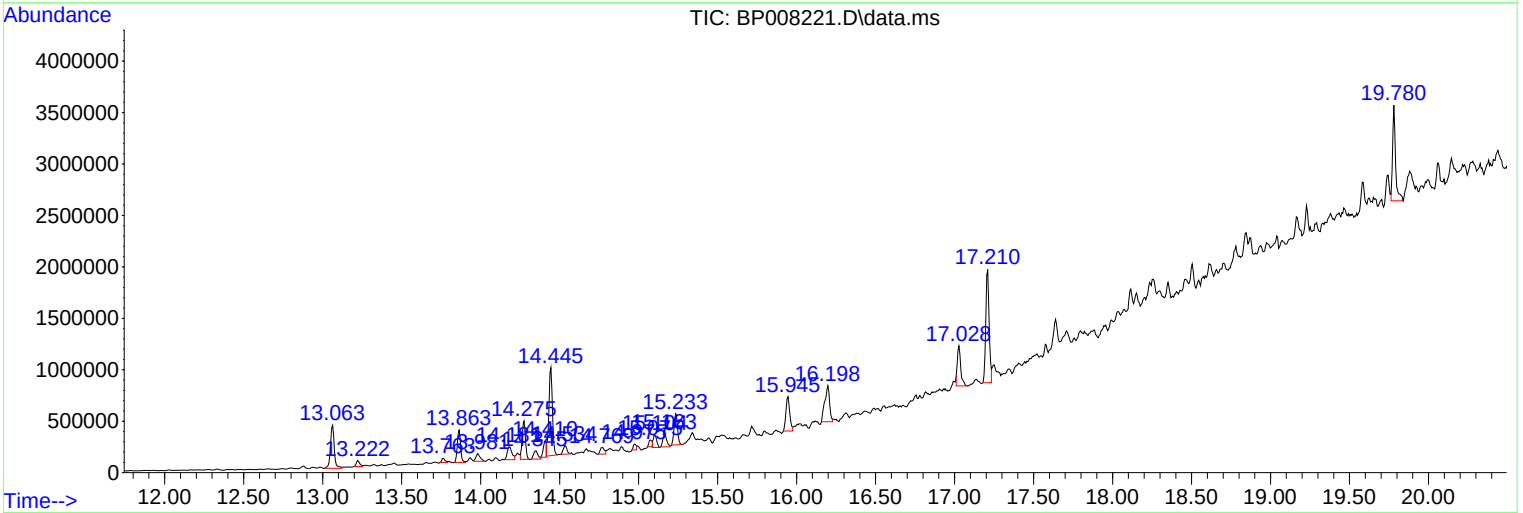
Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

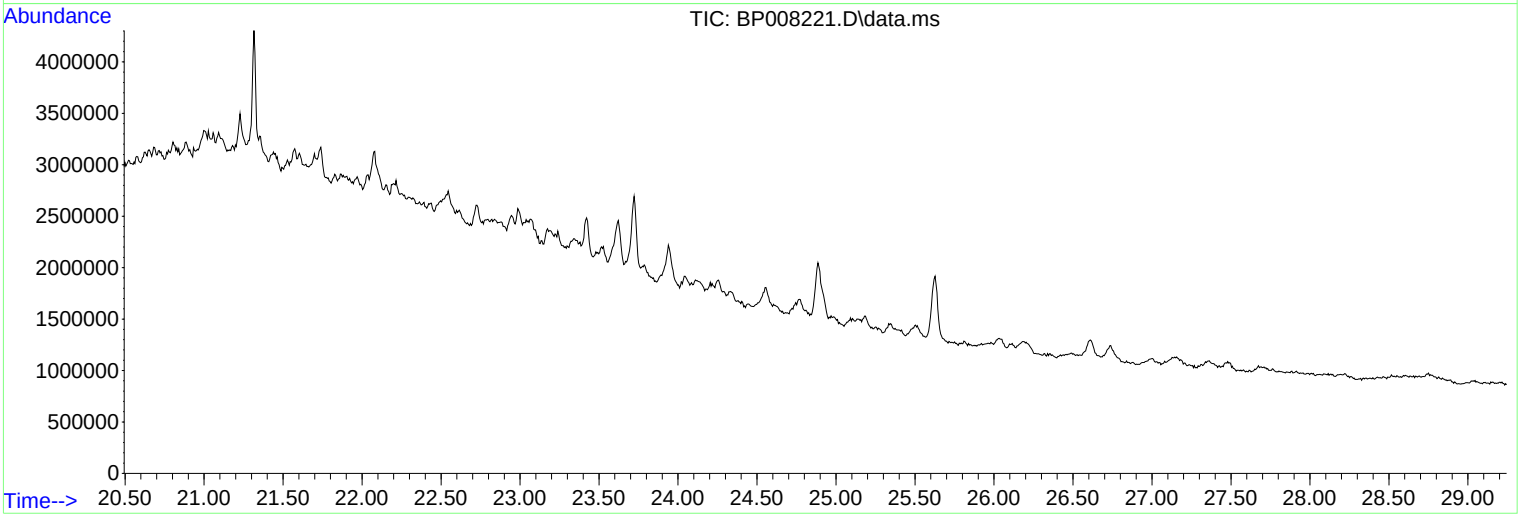
Instrument :
BNA_P
ClientSampleId :
B-2-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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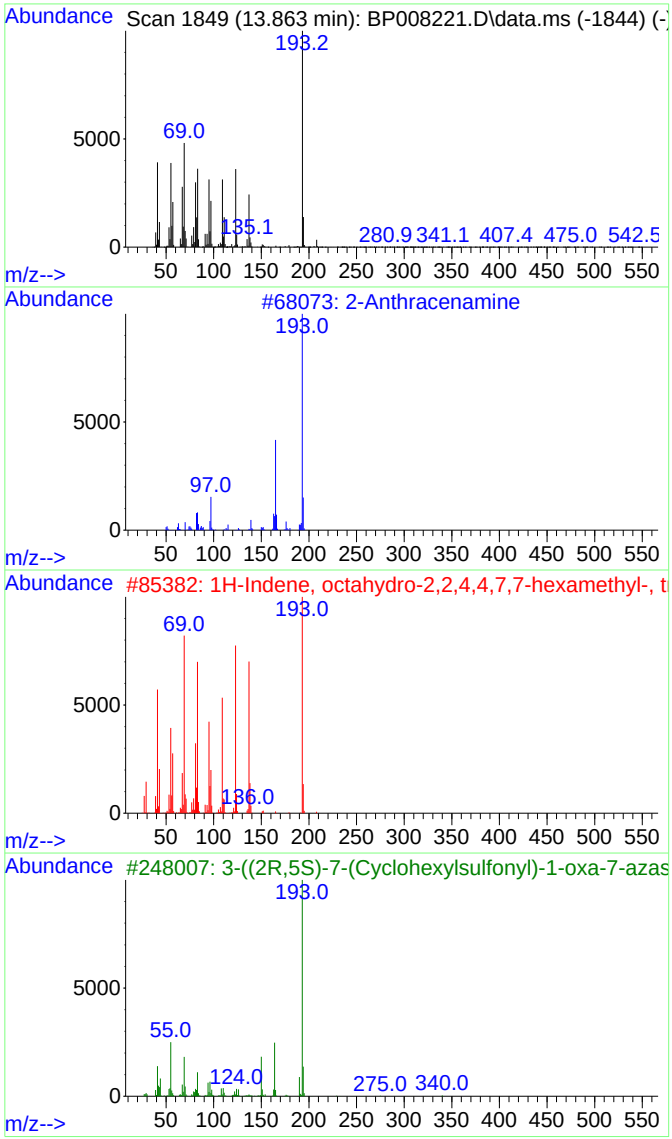
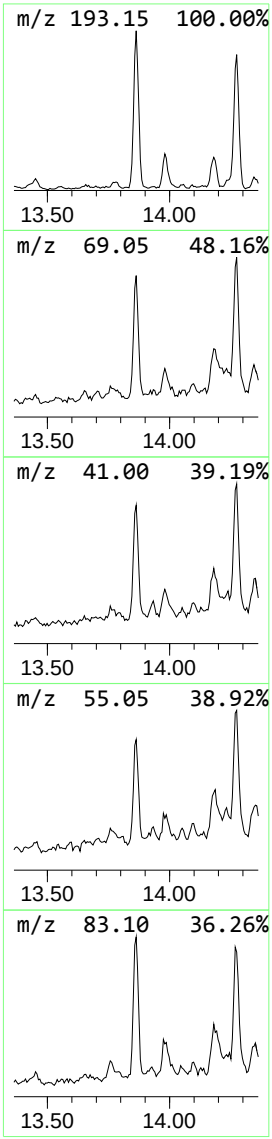
****

Peak Number 2 unknown13.863 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	6.91 ng	457009	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Anthracenamine	193	C14H11N	000613-13-8	38
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	38
3	3-((2R,5S)-7-(Cyclohexylsulfonyl...	340	C17H28N2O3S	1000483-82-6	35
4	1-Anthracenamine	193	C14H11N	000610-49-1	35
5	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35





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Instrument :
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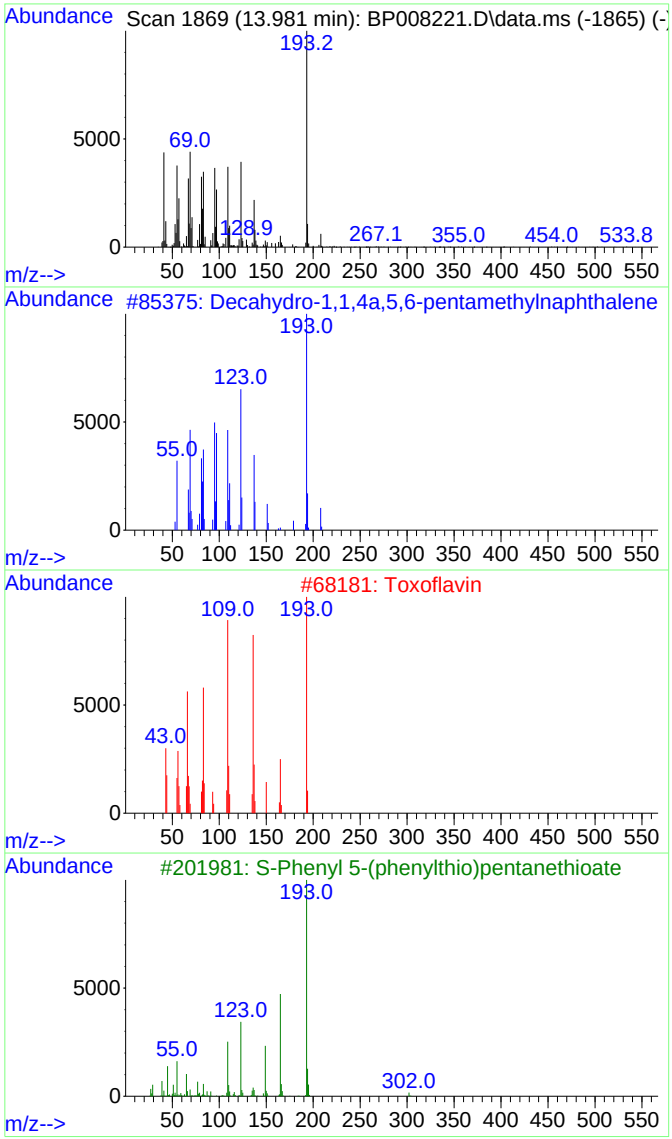
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

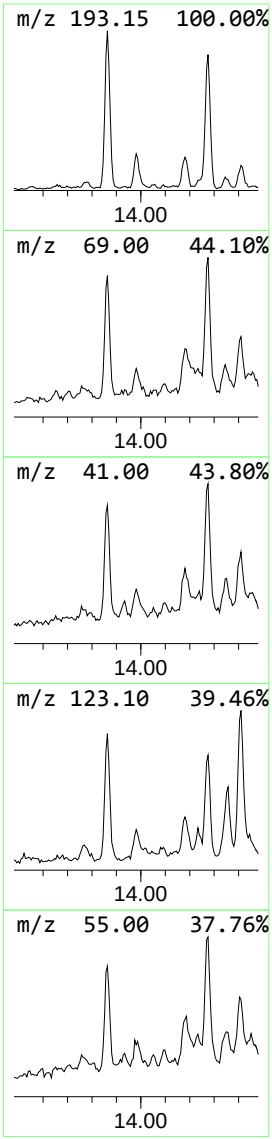
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.981	2.10 ng	139035	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	81
2	Toxoflavin	193	C7H7N5O2	000084-82-2	43
3	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	40
4	trans-3-Methoxy-b-methyl-b-niros...	193	C10H11NO3	018738-95-9	30
5	[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	30





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Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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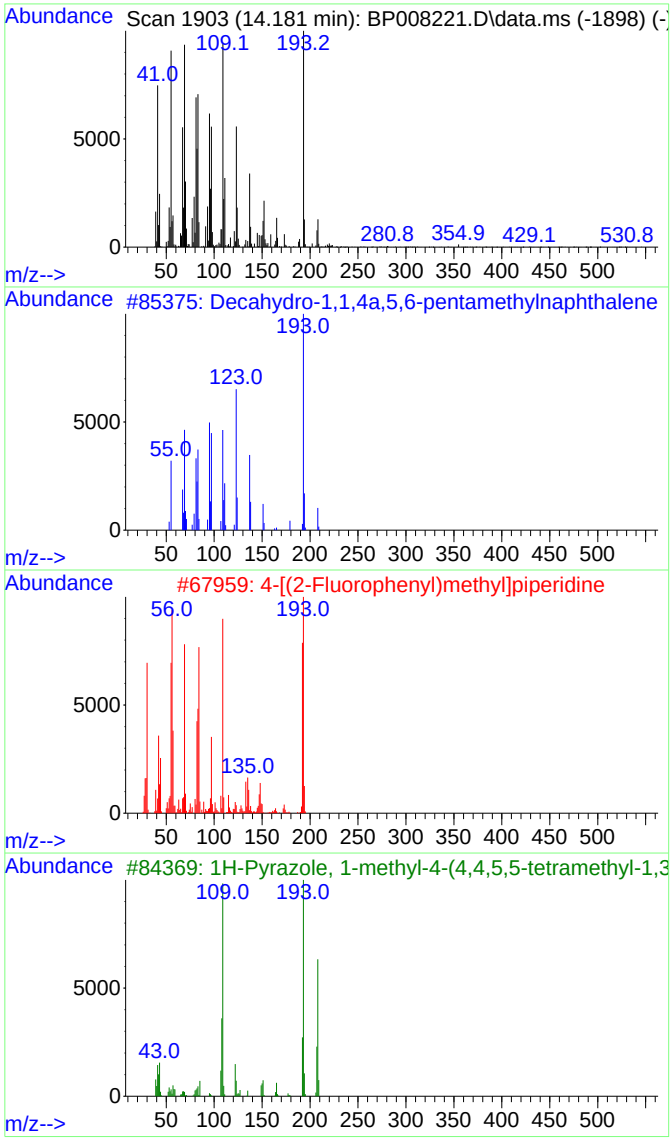
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

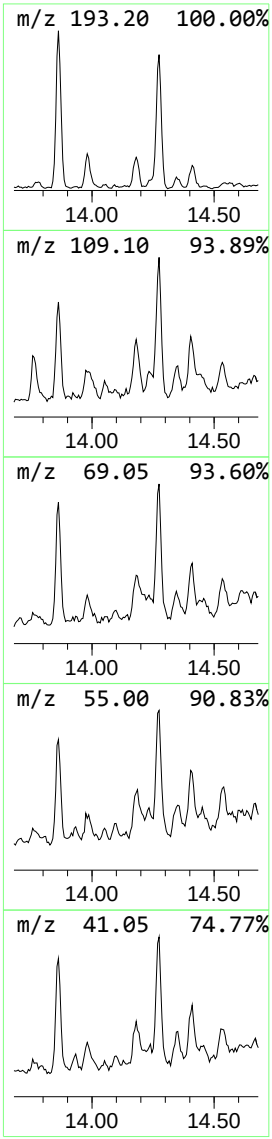
****

Peak Number 4 4-[(2-Fluorophenyl)methyl]p... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.181	4.04 ng	267053	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	93
2	4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	52
3	1H-Pyrazole, 1-methyl-4-(4,4,5,5...	208	C10H17BN2O2	1000319-69-0	46
4	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	43
5	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120321\
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Acq On : 04 Dec 2021 00:13
Operator : CG/JU
Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

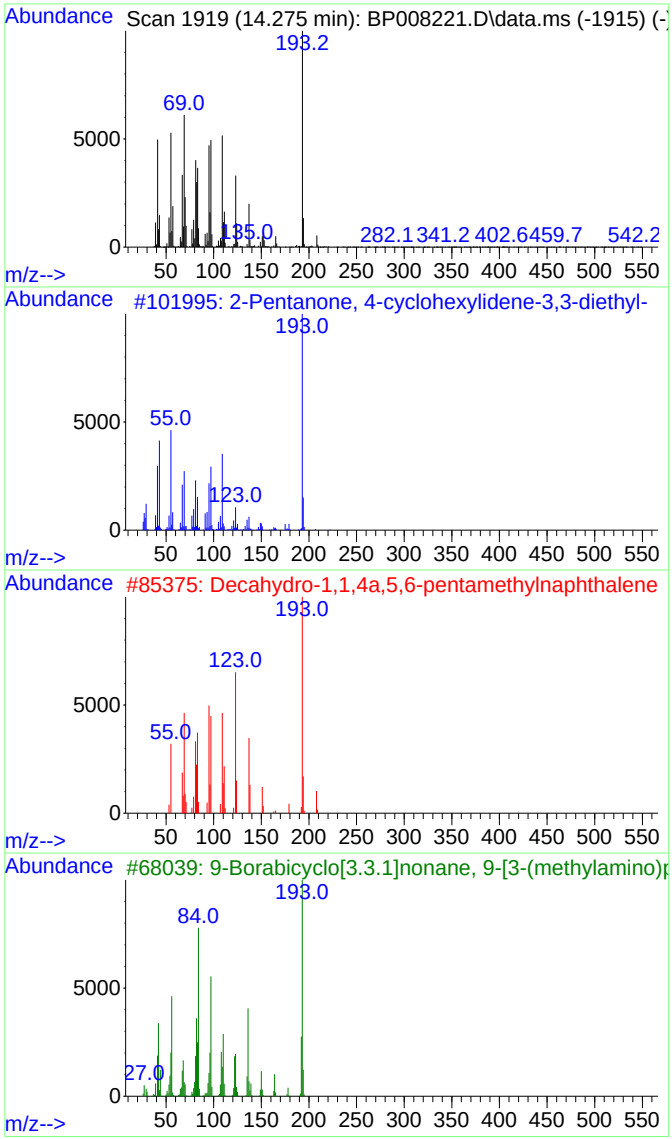
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

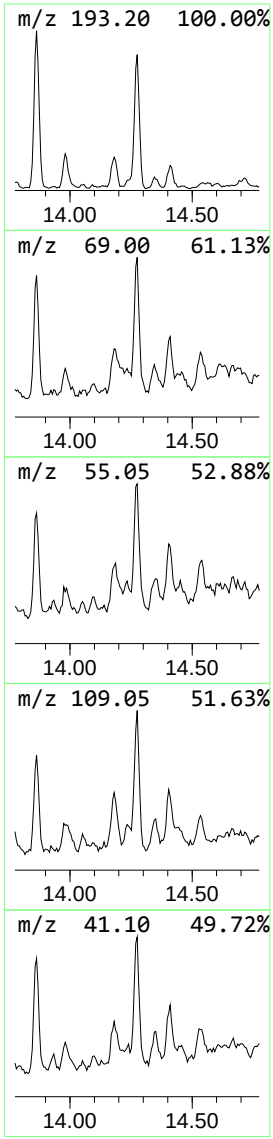
****

Peak Number 5 unknown14.275 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.275	8.05 ng	532844	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
3	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1010162-56-0	43
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
5	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	38





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

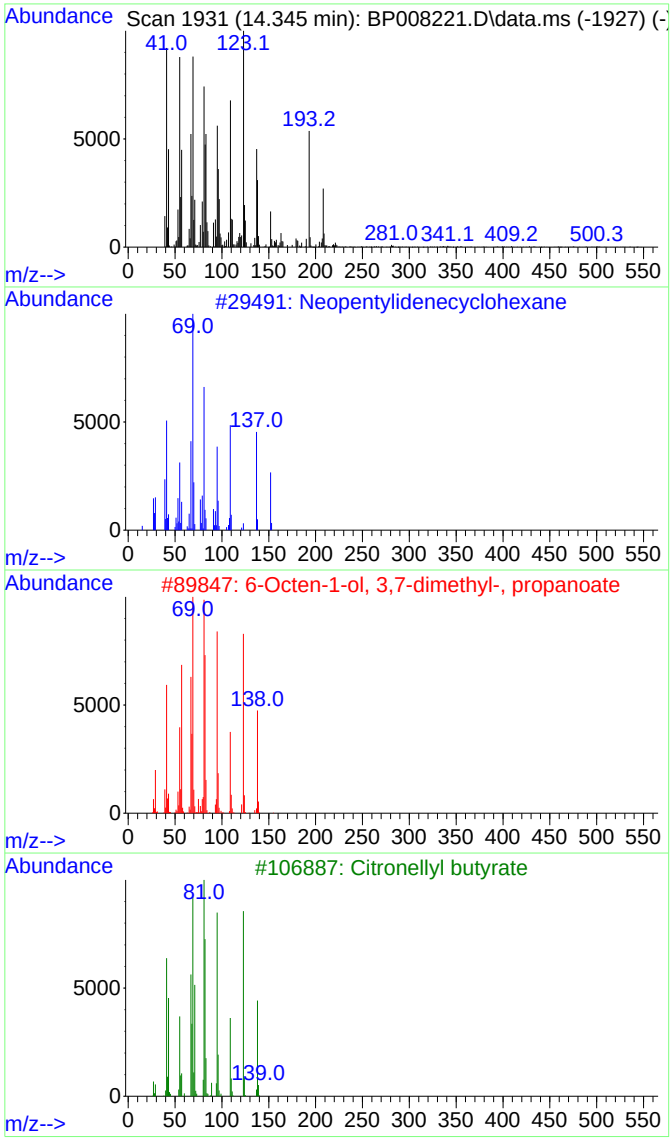
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

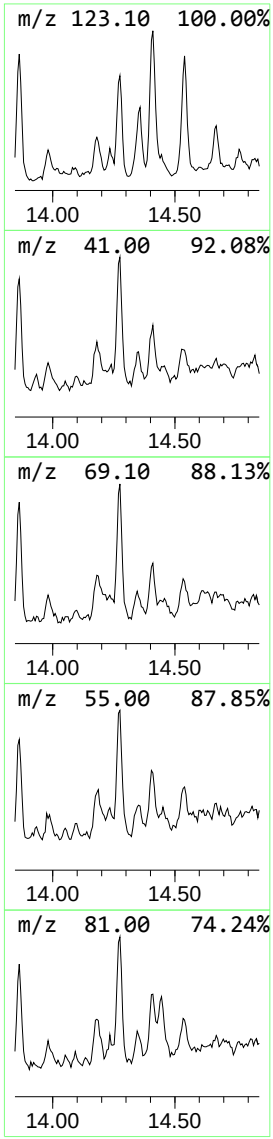
****

Peak Number 6 Neopentylidenecyclohexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	2.30 ng	152509	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentylidenecyclohexane	152	C11H20	039546-80-0	60
2	6-Octen-1-ol, 3,7-dimethyl-, pro...	212	C13H24O2	000141-14-0	53
3	Citronellyl butyrate	226	C14H26O2	000141-16-2	49
4	3,7-Dimethyloct-6-en-1-yl octanoate	282	C18H34O2	072934-05-5	49
5	7-Hexadecyn-1-ol	238	C16H30O	000822-21-9	44





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Misc :
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TIC Library : C:\Database\NIST20.L
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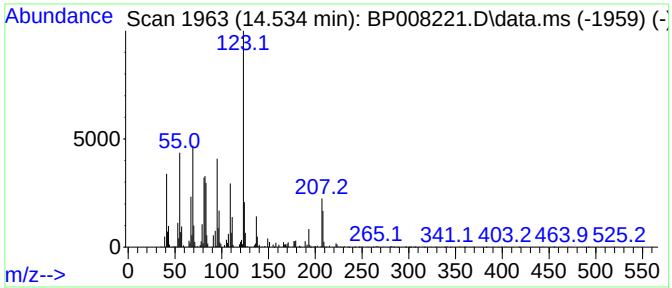
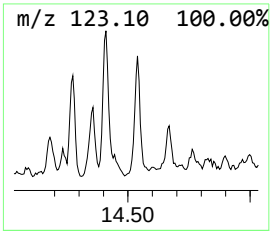
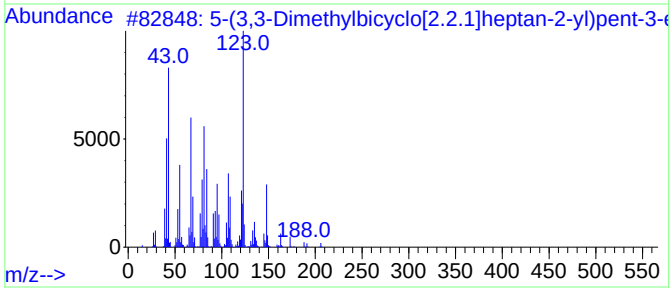
****
Peak Number 7 5-(3,3-Dimethylbicyclo[2.2.... Concentration Rank 11

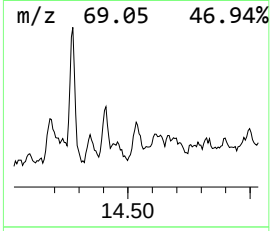
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.534	2.11 ng	139439	Acenaphthene-d10	14.445

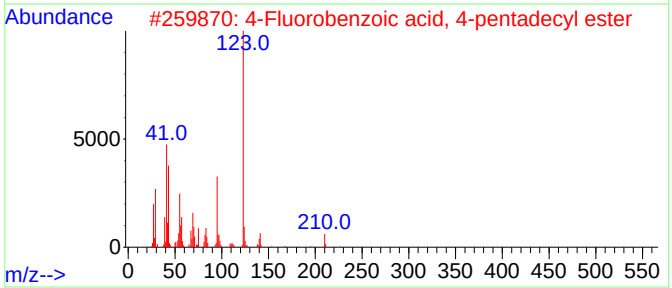
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(3,3-Dimethylbicyclo[2.2.1]hep...	206	C14H22O	1000497-97-7	50
2	4-Fluorobenzoic acid, 4-pentadec...	350	C22H35FO2	1000280-68-5	43
3	3-(2-Ethyl-imidazol-1-yl)-propio...	168	C8H12N2O2	1010277-78-0	43
4	Imidazolidin-2-one, 1-(2-fluorob...	208	C10H9FN2O2	1010310-62-2	43
5	4-Fluorobenzoic acid, 6-ethyl-3-...	280	C17H25FO2	1000279-07-4	43

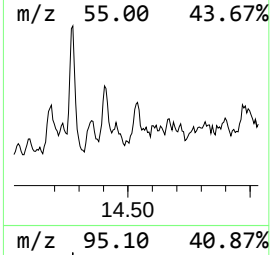


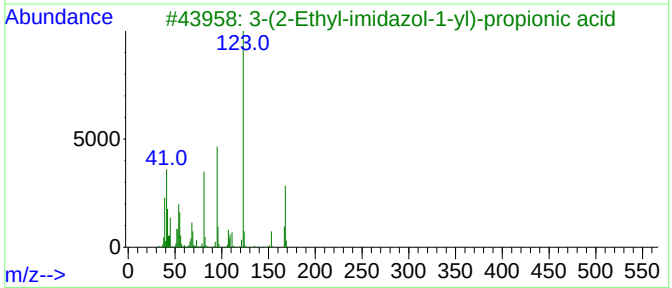


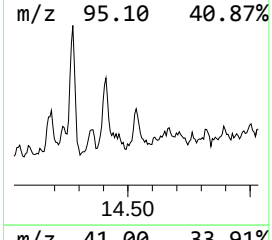


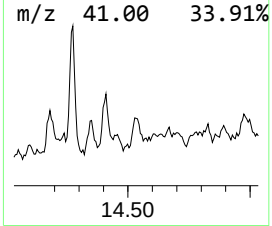












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

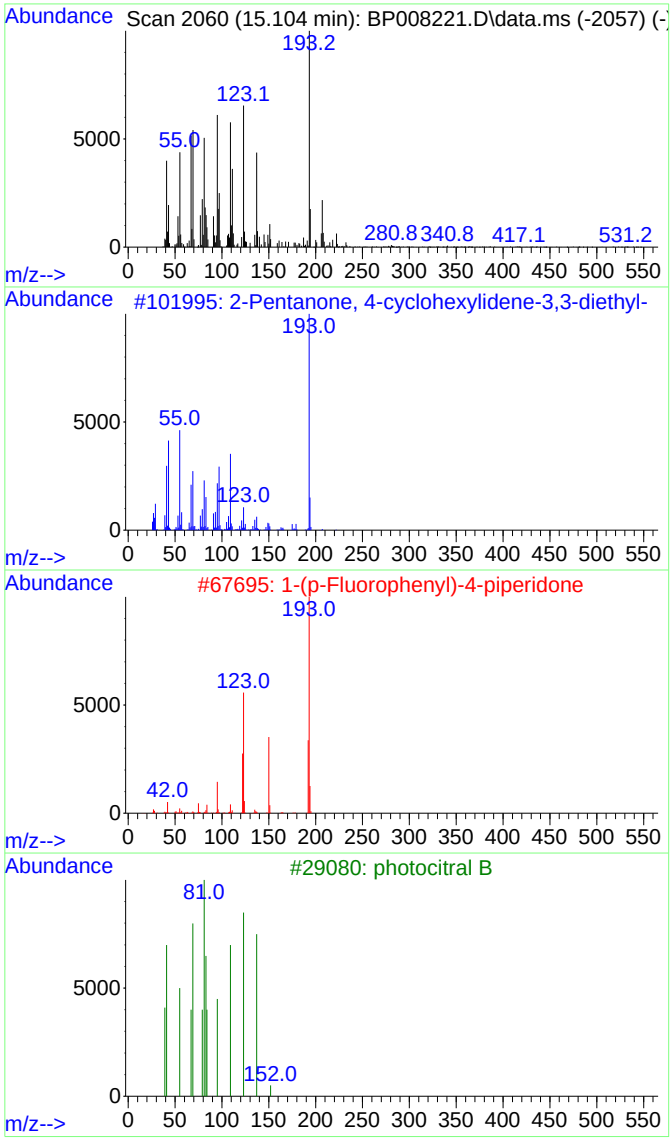
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

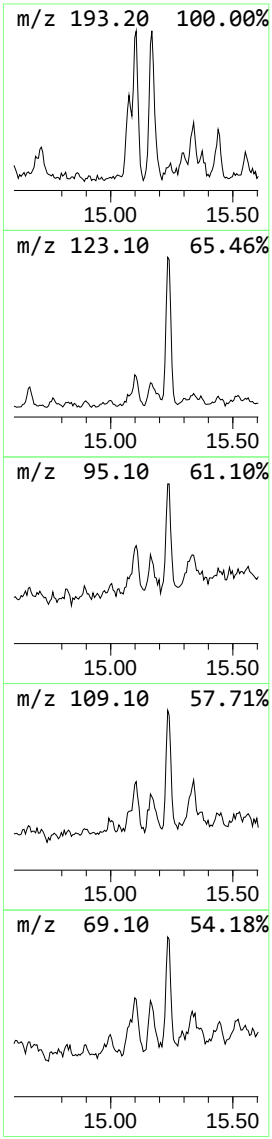
****

Peak Number 8 unknown15.104 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.69 ng	177808	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	35
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
3	photocitral B	152	C10H16O	006040-45-5	27
4	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	22
5	4,5,6,7-Tetrahydro-3-indolinone	137	C8H11NO	058074-25-2	22





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

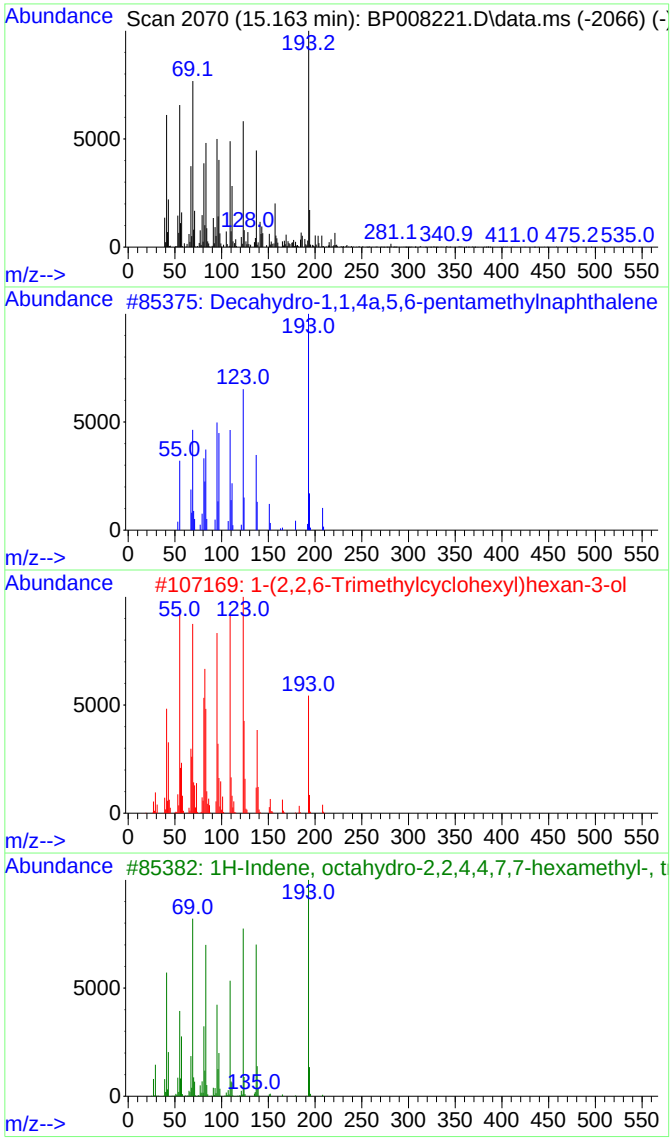
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

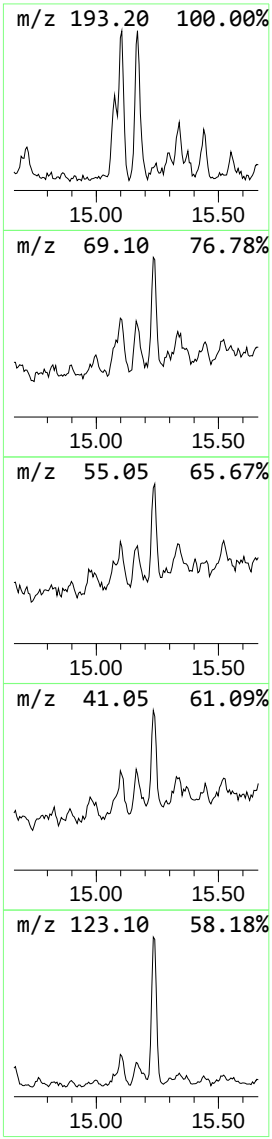
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-(2,2,6-Trimethylcyclohexy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	3.20 ng	211532	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	68
2	1-(2,2,6-Trimethylcyclohexyl)hex...	226	C15H30O	070788-30-6	53
3	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	35
4	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	27
5	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120321\
Data File : BP008221.D
Acq On : 04 Dec 2021 00:13
Operator : CG/JU
Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

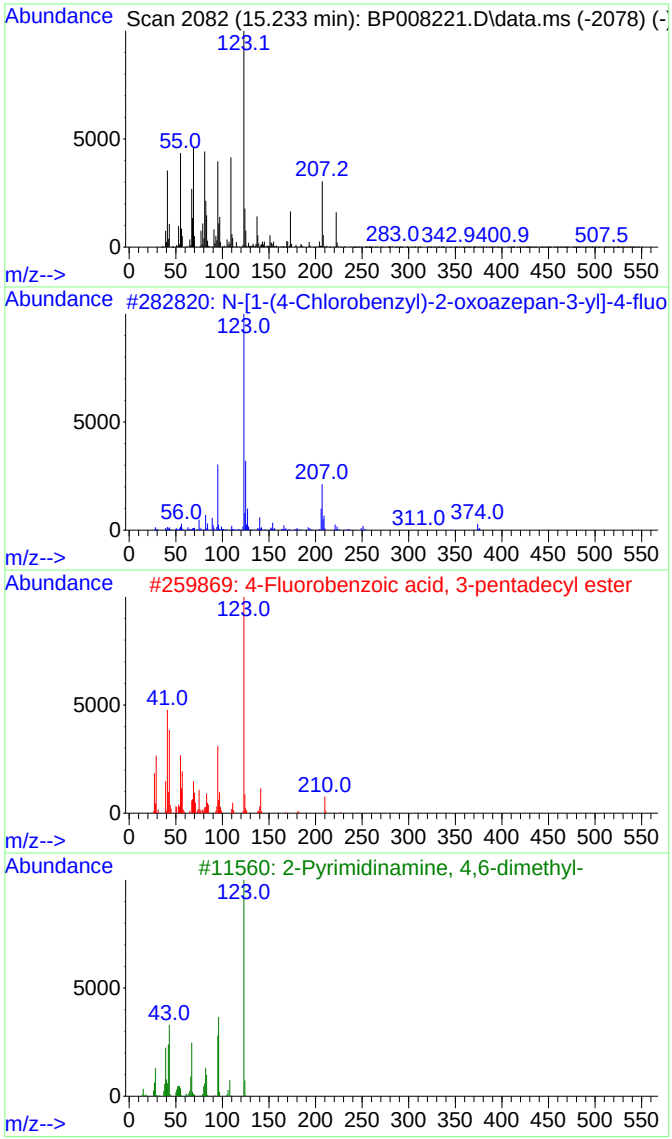
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

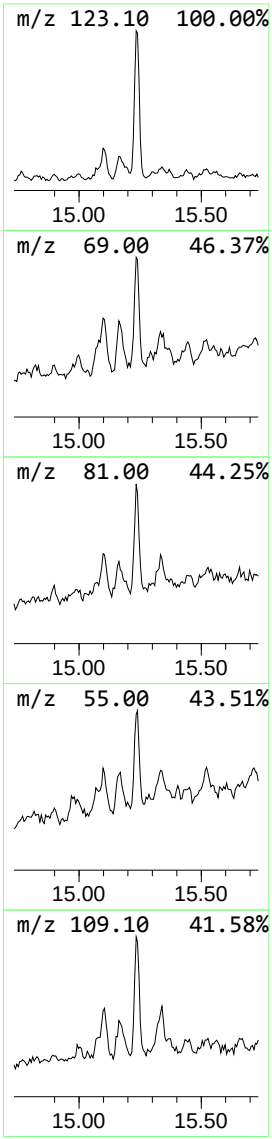
****

Peak Number 10 unknown15.233 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	7.08 ng	468320	Acenaphthene-d10	14.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-[1-(4-Chlorobenzyl)-2-oxoazepa...	374	C20H20ClFN2O2	1000481-70-9	47
2	4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	47
3	2-Pyrimidinamine, 4,6-dimethyl-	123	C6H9N3	000767-15-7	46
4	4-Nitrophenyl bicyclo[4.1.0]hept...	261	C14H15NO4	328938-65-4	46
5	1-(4-Fluorobenzoyl)piperazine	208	C11H13FN2O	102391-98-0	43





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Data File : BP008221.D
Acq On : 04 Dec 2021 00:13
Operator : CG/JU
Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

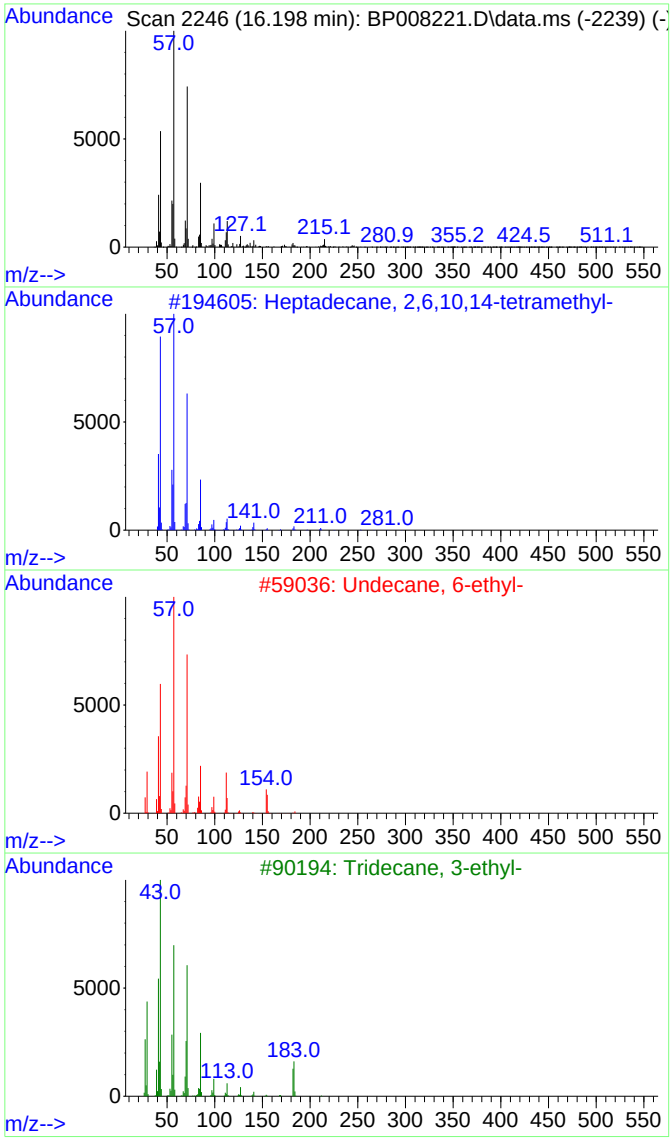
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

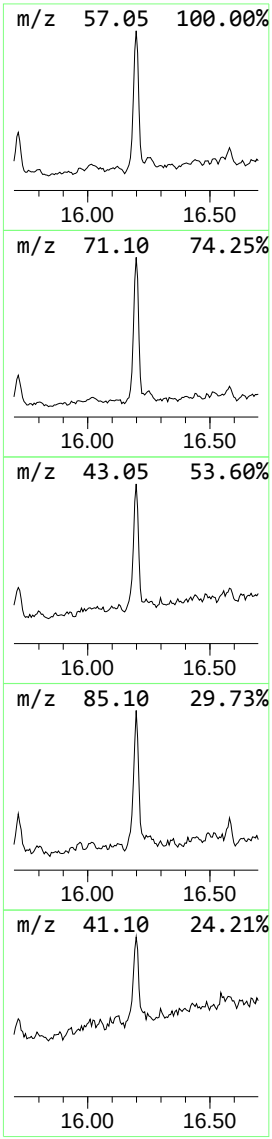
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Heptadecane, 2,6,10,14-tetr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.198	8.84 ng	729025	Phenanthrene-d10	17.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	91
2	Undecane, 6-ethyl-	184	C13H28	017312-60-6	87
3	Tridecane, 3-ethyl-	212	C15H32	013286-73-2	87
4	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	86





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Data File : BP008221.D
Acq On : 04 Dec 2021 00:13
Operator : CG/JU
Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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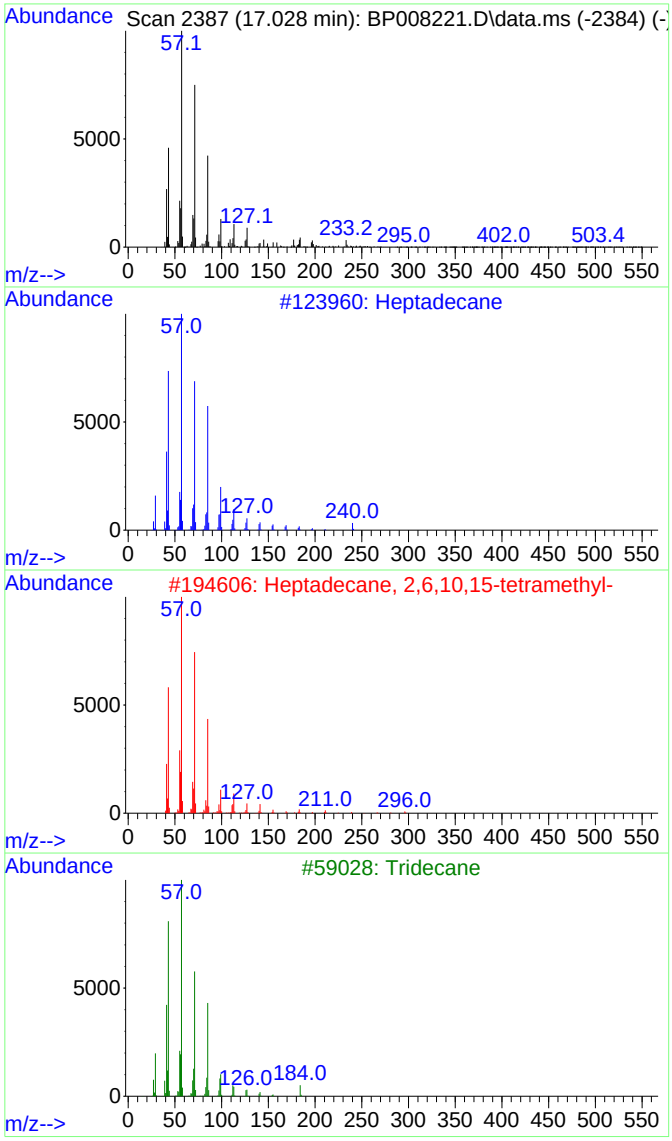
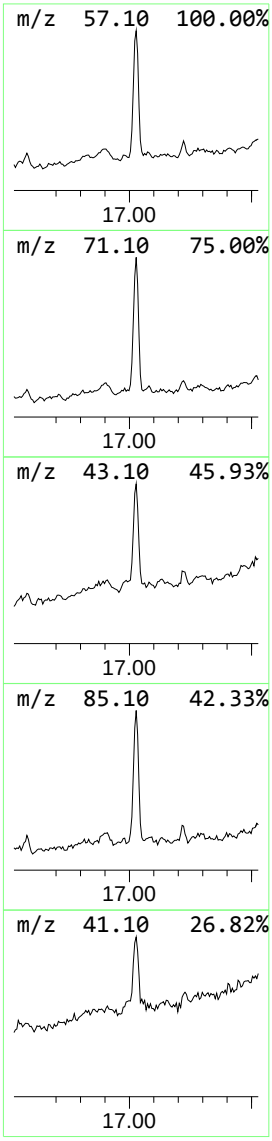
Peak Number 12 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.028	7.03 ng	579891	Phenanthrene-d10	17.210

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3	Tridecane	184	C13H28	000629-50-5	87
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120321\
Data File : BP008221.D
Acq On : 04 Dec 2021 00:13
Operator : CG/JU
Sample : M4915-03 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B-2-10-15

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown13.863	13.863	6.9	ng	457009	3	14.445	1323650	20.0
Decahydro-1,1,4...	13.981	2.1	ng	139035	3	14.445	1323650	20.0
4-[(2-Fluorophe...	14.181	4.0	ng	267053	3	14.445	1323650	20.0
unknown14.275	14.275	8.1	ng	532844	3	14.445	1323650	20.0
Neopentylidenec...	14.345	2.3	ng	152509	3	14.445	1323650	20.0
5-(3,3-Dimethyl...	14.534	2.1	ng	139439	3	14.445	1323650	20.0
unknown15.104	15.104	2.7	ng	177808	3	14.445	1323650	20.0
1-(2,2,6-Trimet...	15.163	3.2	ng	211532	3	14.445	1323650	20.0
unknown15.233	15.233	7.1	ng	468320	3	14.445	1323650	20.0
Heptadecane, 2,...	16.198	8.8	ng	729025	4	17.210	1649340	20.0
Heptadecane	17.028	7.0	ng	579891	4	17.210	1649340	20.0