LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005125.D
Acq On : 31 Mar 2021 14:29
Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : IG004

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-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005125.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.858	295	301	312	rBV	59823	86321	3.65%	0.650%
2	5.317	370	379	394	rBV	863564	1249576	52.90%	9.402%
3	6.899	639	648	659	rBV	826009	1307728	55.36%	9.840%
4	7.716	779	787	793	rBV	131387	212532	9.00%	1.599%
5	8.875	973	984	993	rBV	504510	829993	35.14%	6.245%
6	10.505	1253	1261	1269	rBV	178224	293443	12.42%	2.208%
7	12.987	1675	1683	1692	rBV	1260342	1840331	77.90%	13.847%
8	13.828	1821	1826	1836	rVB2	16151	35120	1.49%	0.264%
9	14.369	1910	1918	1925	rBV	262669	390105	16.51%	2.935%
10	15.869	2162	2173	2181	rBV	1112927	1578475	66.82%	11.877%
11	16.528	2279	2285	2295	rBV3	28003	53013	2.24%	0.399%
12	17.128	2379	2387	2392	rBV	321515	451476	19.11%	3.397%
13	17.516	2448	2453	2458	rBV2	36939	54473	2.31%	0.410%
14	17.910	2516	2520	2527	rBV5	18435	24087	1.02%	0.181%
15	18.028	2535	2540	2548	rBV2	252123	335095	14.19%	2.521%
16	18.922	2689	2692	2697	rVB2	58642	68513	2.90%	0.516%
17	19.151	2728	2731	2734	rBV4	23274	40568	1.72%	0.305%
18	19.263	2747	2750	2755	rBV	109172	134968	5.71%	1.016%
19	19.704	2819	2825	2830	rBV	2027966	2362293	100.00%	17.775%
20	20.939	3031	3035	3040	rBV2	203681	304014	12.87%	2.288%
21	21.222	3079	3083	3091	rBV	399619	539456	22.84%	4.059%
22	21.492	3126	3129	3135	rVB	96031	135825	5.75%	1.022%
23	22.004	3212	3216	3223	rVB	309643	479669	20.31%	3.609%
24	23.510	3468	3472	3480	rVB	253787	482962	20.44%	3.634%

Sum of corrected areas: 13290036

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Misc :
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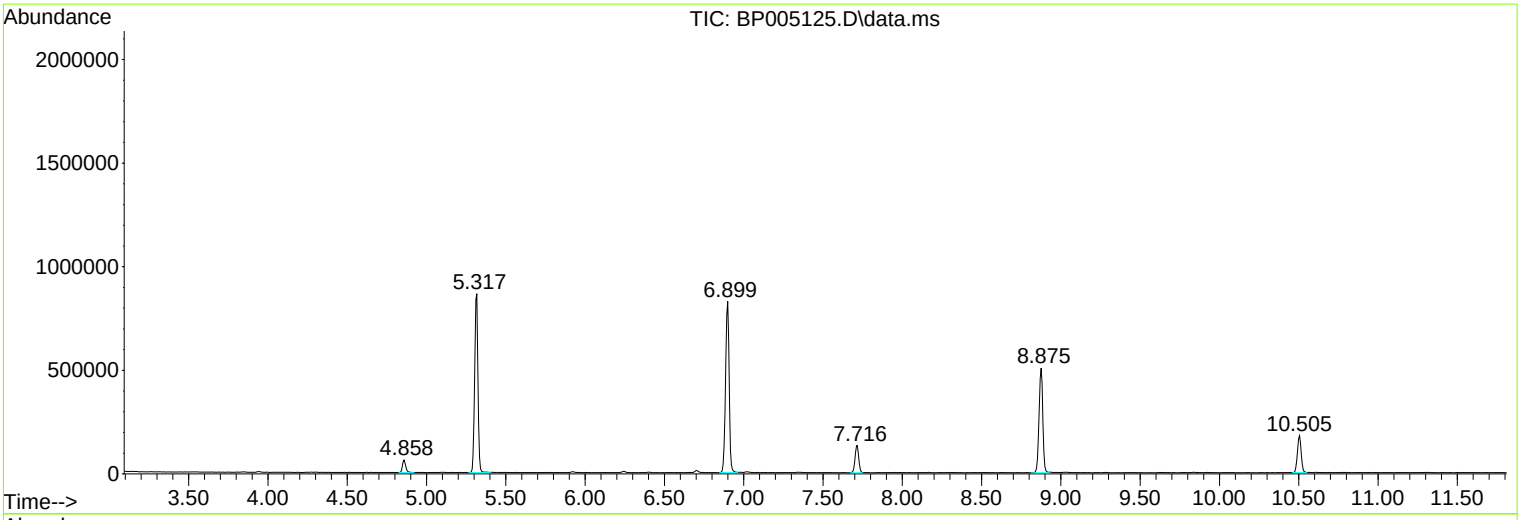
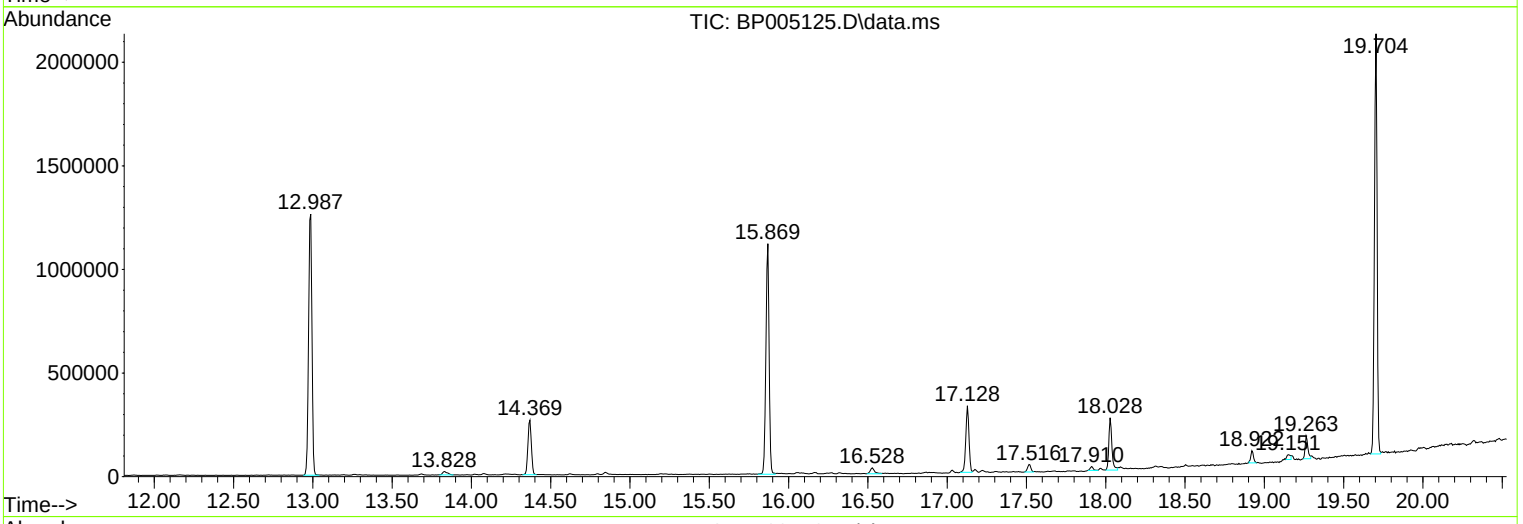
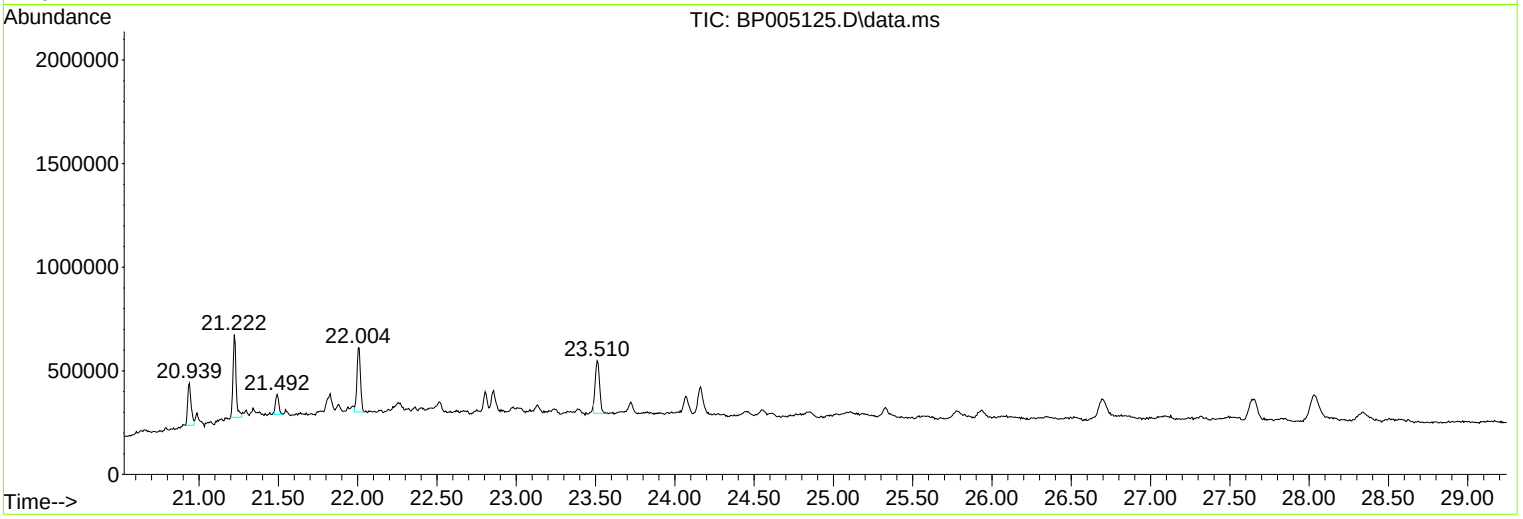
Instrument :
BNA_P
ClientSampleId :
IG004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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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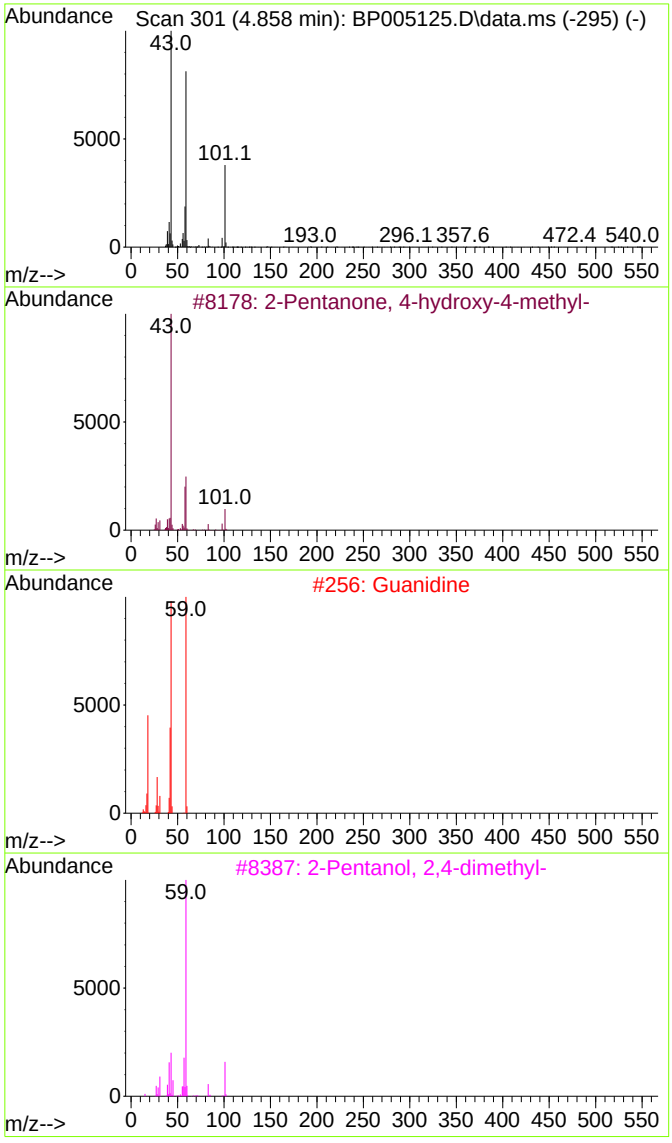
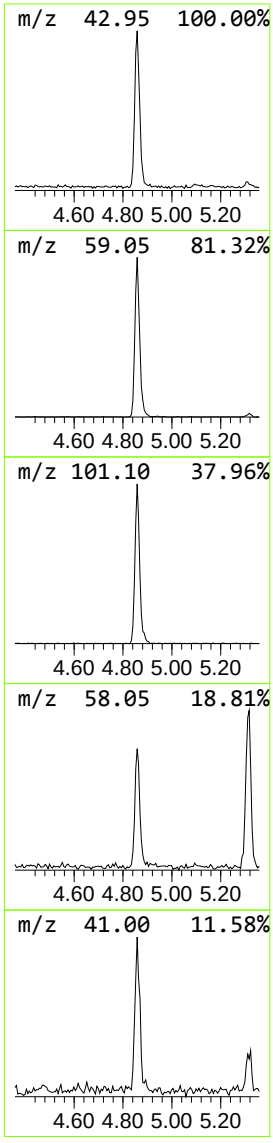
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.858	8.12 ng	86321	1,4-Dichlorobenzene-d4	7.711

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Guanidine	59	CH5N3	000113-00-8	50
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	38
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	37
5	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	36





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Data File : BP005125.D
Acq On : 31 Mar 2021 14:29
Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : IG004

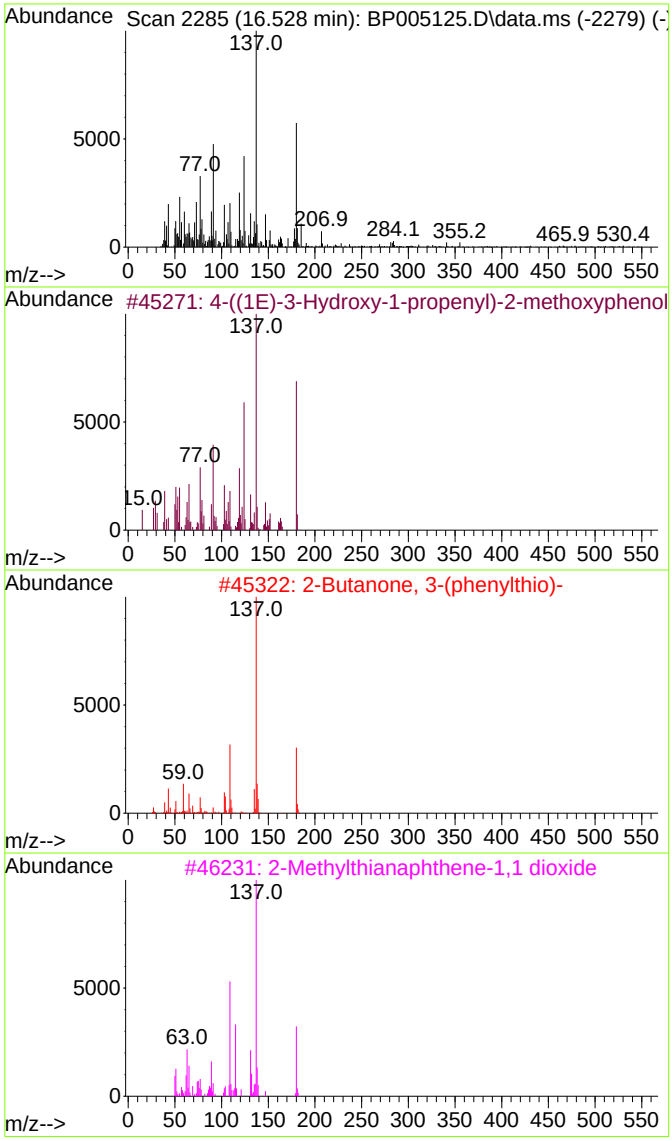
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

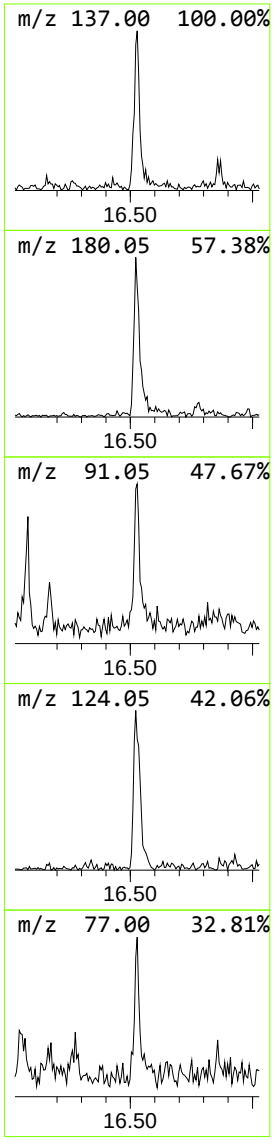
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 4-((1E)-3-Hydroxy-1-propeny... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.528	2.35 ng	53013	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-((1E)-3-Hydroxy-1-propenyl)-2-...	180	C10H12O3	1000297-95-5	70
2	2-Butanone, 3-(phenylthio)-	180	C10H12OS	013023-53-5	46
3	2-Methylthianaphthene-1,1 dioxide	180	C9H8O2S	006224-55-1	46
4	(+)-s-2-Phenethanamine, 1-methyl...	271	C17H21NO2	1000127-89-6	38
5	5-(Acetylaminomethyl)-4-amino-2-...	180	C8H12N4O	023676-63-3	38





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Acq On : 31 Mar 2021 14:29
Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
IG004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
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TIC Library : C:\DATABASE\NIST11.L
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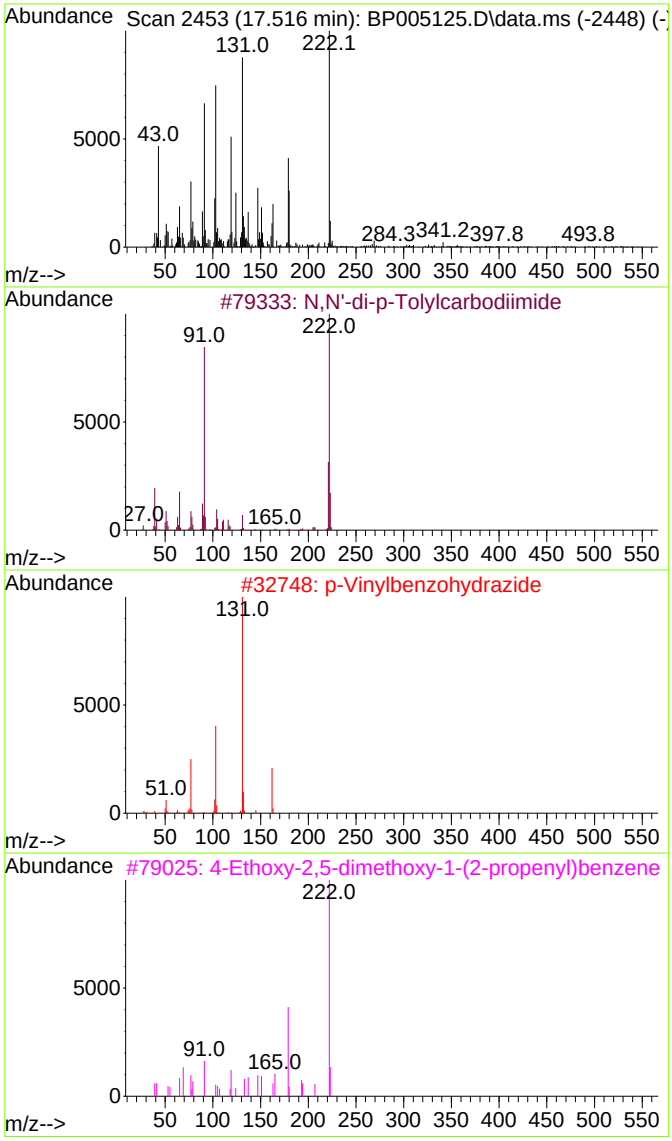
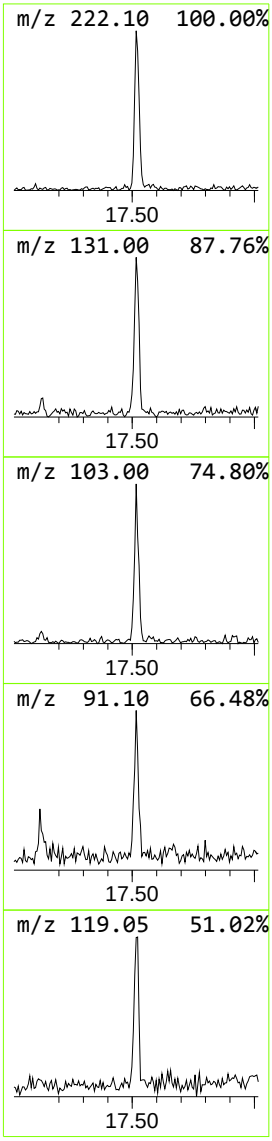
Peak Number 3 unknown17.51 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.516	2.41 ng	54473	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N'-di-p-Tolylcarbodiimide	222	C15H14N2	000726-42-1	44
2	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	27
3	4-Ethoxy-2,5-dimethoxy-1-(2-prop...	222	C13H18O3	1000122-67-4	25
4	trans-2,5-Dimethoxy-4-ethoxy-.be...	222	C13H18O3	1000122-68-2	25
5	7-Oxo-1,3,5-cycloheptatriene-1-c...	131	C8H5NO	000934-19-0	25





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Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : IG004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

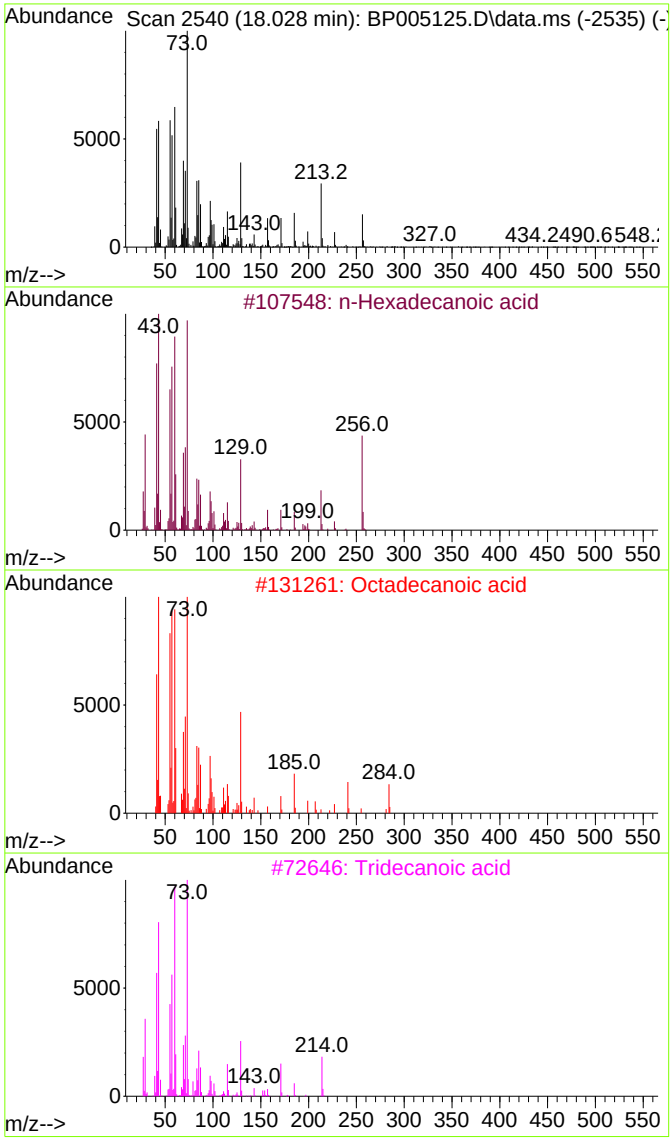
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

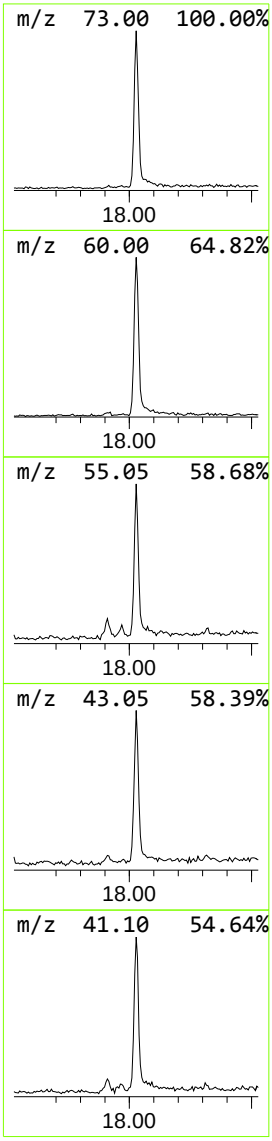
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.028	14.84 ng	335095	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Octadecanoic acid	284	C18H36O2	000057-11-4	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005125.D
Acq On : 31 Mar 2021 14:29
Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
IG004

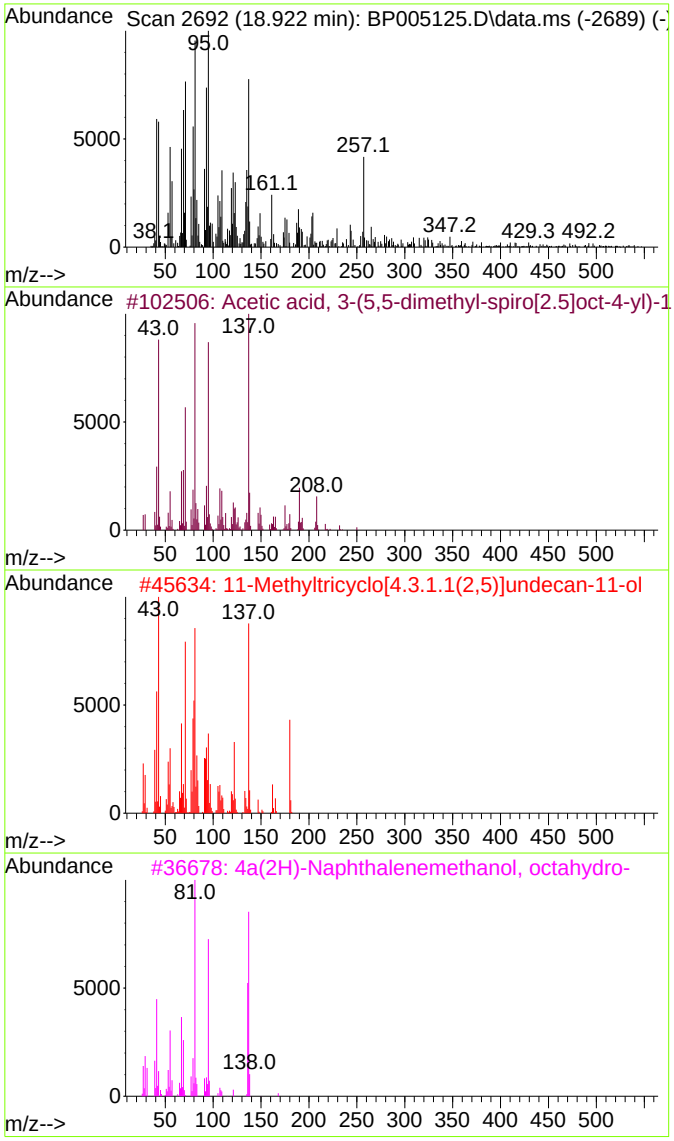
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

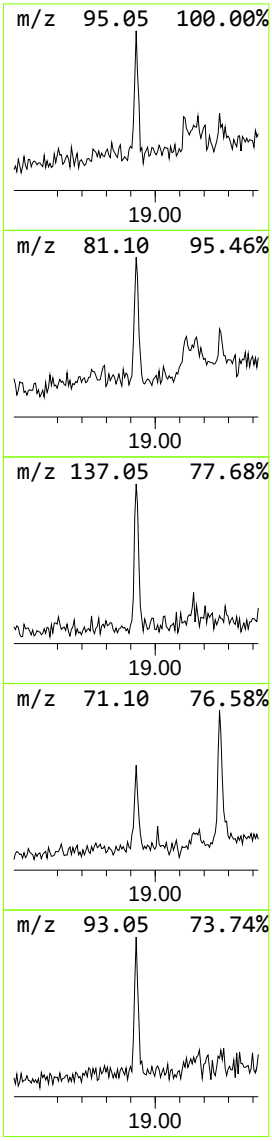
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Acetic acid, 3-(5,5-dimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.922	3.04 ng	68513	Phenanthrene-d10	17.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 3-(5,5-dimethyl-spi...	250	C16H26O2	077143-33-0	53
2	11-Methyltricyclo[4.3.1.1(2,5)]u...	180	C12H20O	174226-52-9	43
3	4a(2H)-Naphthalenemethanol, octa...	168	C11H20O	099992-19-5	38
4	3,5-Octadiene, 4,5-diethyl-	166	C12H22	067652-84-0	38
5	trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	38





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Operator : CG/JU
Sample : M1832-04
Misc :
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Instrument : BNA_P
ClientSampleId : IG004

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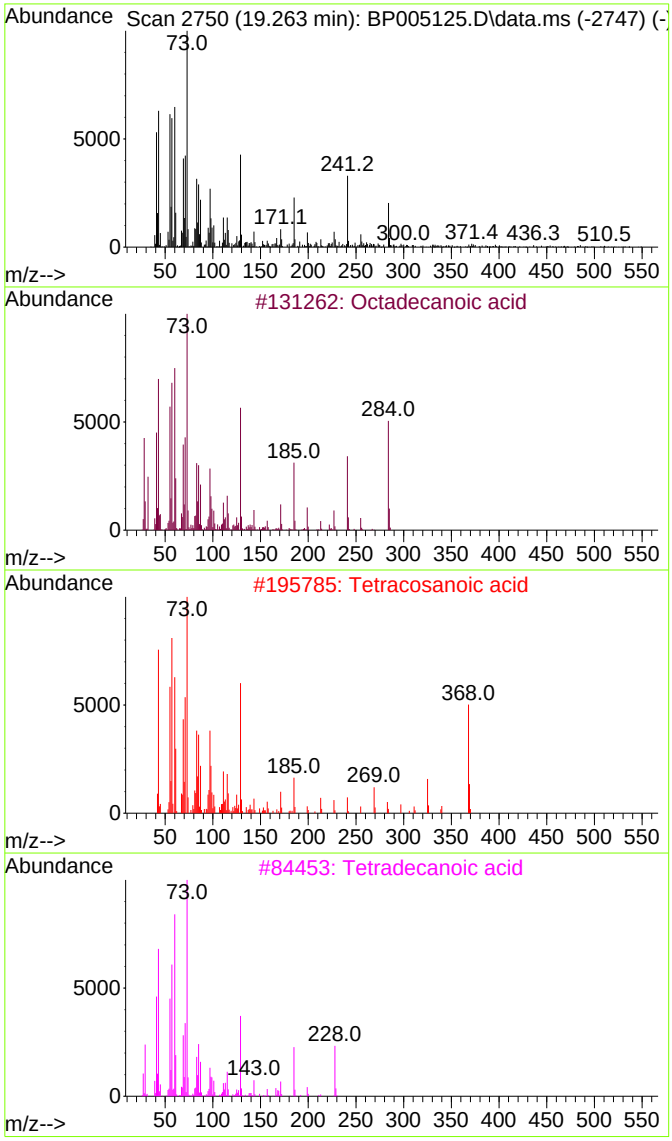
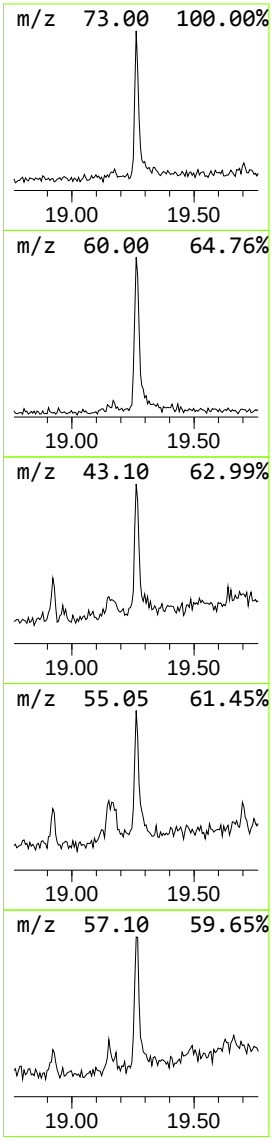
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.263	5.00 ng	134968	Chrysene-d12	21.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetracosanoic acid	368	C24H48O2	000557-59-5	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	59





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Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
IG004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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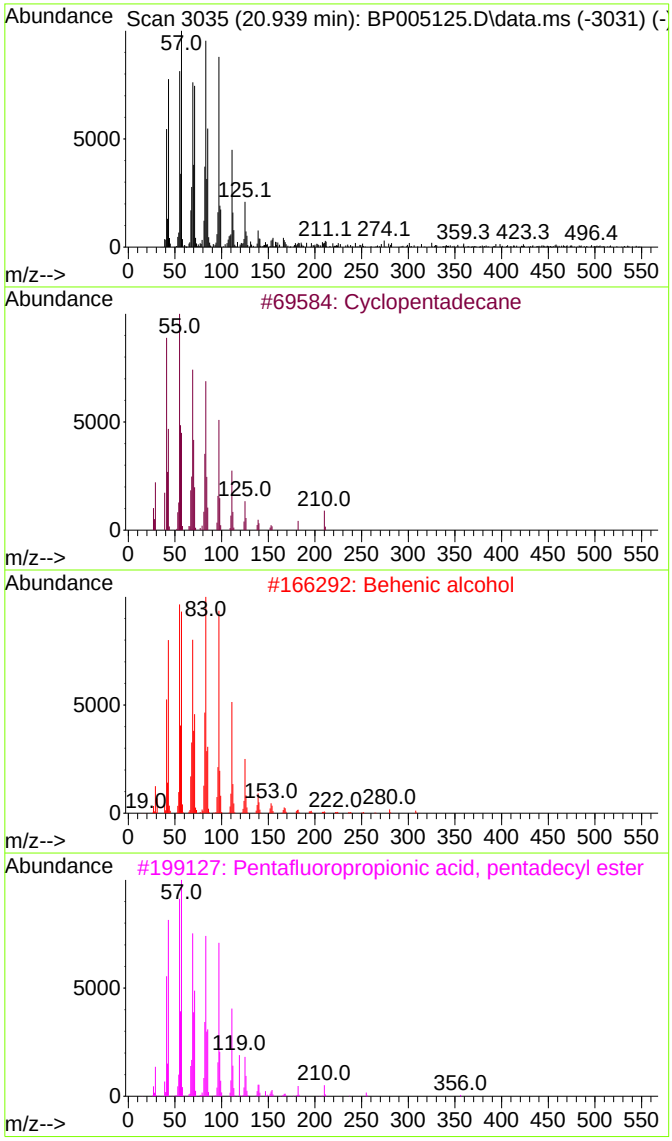
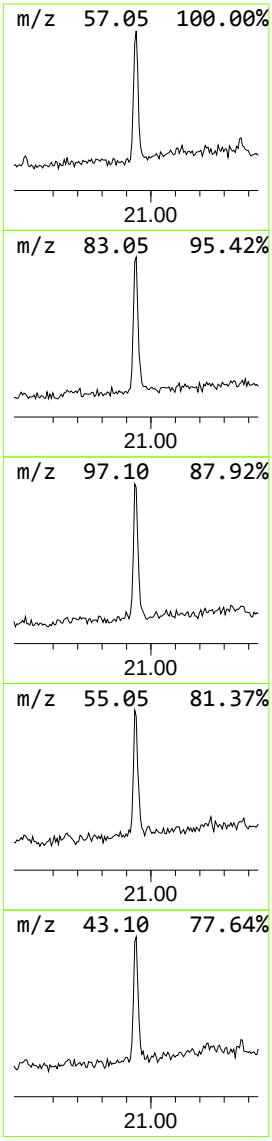
Peak Number 7 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.939	11.27 ng	304014	Chrysene-d12	21.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87





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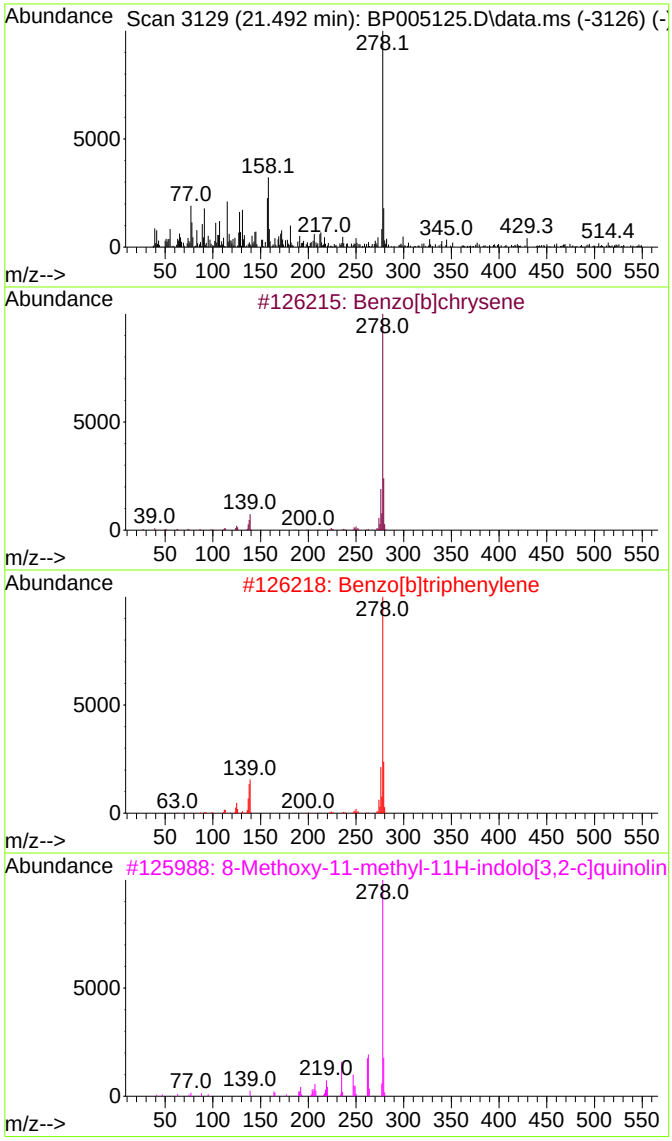
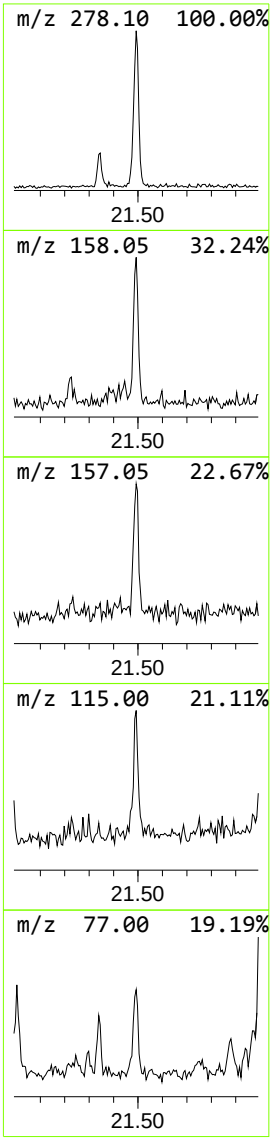
Peak Number 8 Benzo[b]chrysene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.492	5.04 ng	135825	Chrysene-d12	21.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]chrysene	278	C22H14	000214-17-5	64
2	Benzo[b]triphenylene	278	C22H14	000215-58-7	64
3	8-Methoxy-11-methyl-11H-indolo[3...	278	C17H14N2O2	116618-53-2	64
4	Benzo[a]naphthacene	278	C22H14	000226-88-0	64
5	1,4-Pentadien-3-one, 1-(1,3-benz...	278	C18H14O3	1000319-47-3	64





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Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : IG004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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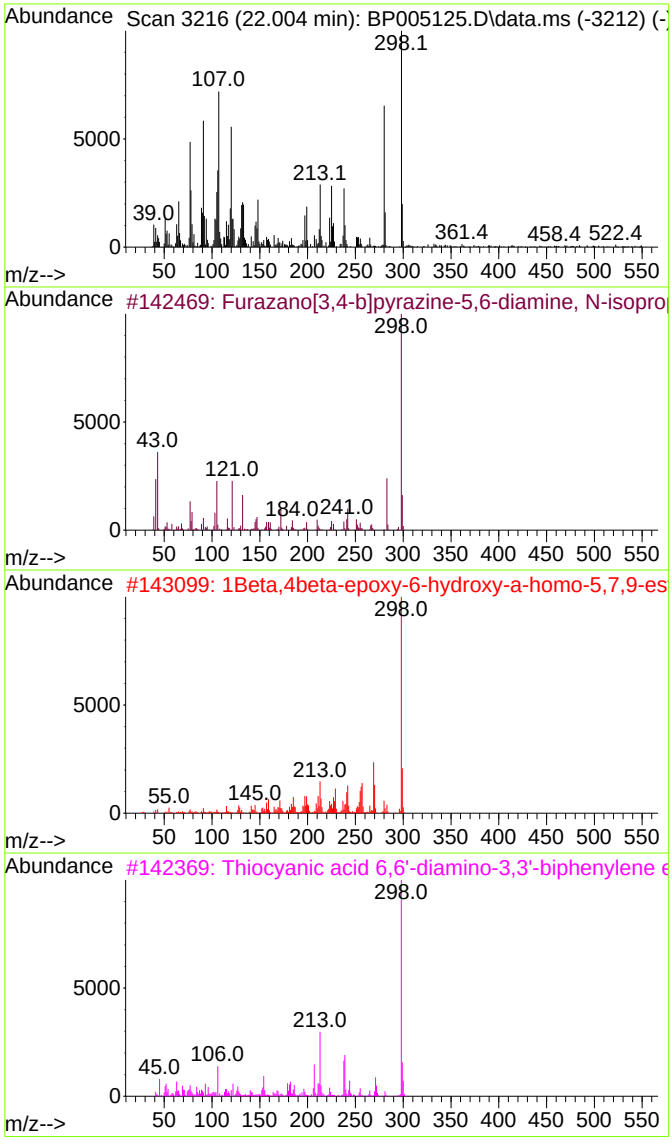
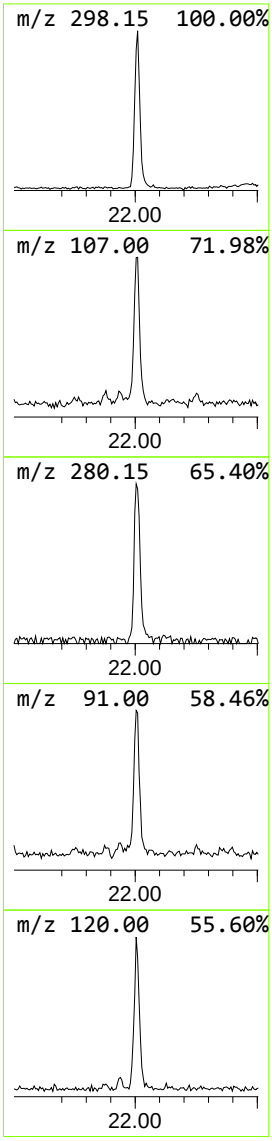
****

Peak Number 9 unknown22.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.004	17.78 ng	479669	Chrysene-d12	21.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furazano[3,4-b]pyrazine-5,6-diam...	298	C15H18N6O	309731-58-6	42
2	1Beta,4beta-epoxy-6-hydroxy-a-ho...	298	C19H22O3	1000240-12-7	38
3	Thiocyanic acid 6,6'-diamino-3,3...	298	C14H10N4S2	1000251-84-7	30
4	Acenaphtho[1,2-b]quinoxaline-9-c...	298	C19H10N2O2	134859-13-5	27
5	5-Pregnen-3.beta.-ol-20-one, tri...	412	C23H31F3O3	1000352-61-4	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP033121\
Data File : BP005125.D
Acq On : 31 Mar 2021 14:29
Operator : CG/JU
Sample : M1832-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : IG004

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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-...	4.858	8.1	ng	86321	1	7.711	212532	20.0
4-((1E)-3-Hydro...	16.528	2.4	ng	53013	4	17.128	451476	20.0
unknown17.51	17.516	2.4	ng	54473	4	17.128	451476	20.0
n-Hexadecanoic ...	18.028	14.8	ng	335095	4	17.128	451476	20.0
Acetic acid, 3-...	18.922	3.0	ng	68513	4	17.128	451476	20.0
Octadecanoic acid	19.263	5.0	ng	134968	5	21.222	539456	20.0
Cyclopentadecane	20.939	11.3	ng	304014	5	21.222	539456	20.0
Benzo[b]chrysene	21.492	5.0	ng	135825	5	21.222	539456	20.0
unknown22.00	22.004	17.8	ng	479669	5	21.222	539456	20.0