

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
 Data File : BP005578.D
 Acq On : 15 May 2021 20:36
 Operator : CG/JU
 Sample : M2383-12
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DUP-02-05122021

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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: BP005578.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.264	365	370	387	rBV	92712	159770	8.85%	2.150%
2	6.875	638	644	660	rBV2	42533	92883	5.15%	1.250%
3	7.669	771	779	787	rBV	48976	77534	4.30%	1.043%
4	8.199	864	869	878	rVB	29347	49487	2.74%	0.666%
5	8.840	971	978	991	rVB	161975	276735	15.33%	3.723%
6	10.457	1243	1253	1257	rBV	59799	102305	5.67%	1.376%
7	10.510	1257	1262	1271	rVB	410531	663207	36.74%	8.923%
8	10.634	1278	1283	1294	rVB	12356	23452	1.30%	0.316%
9	12.134	1531	1538	1548	rBV	75125	120621	6.68%	1.623%
10	12.351	1565	1575	1584	rBV	47436	80099	4.44%	1.078%
11	12.940	1666	1675	1686	rBV	589691	831952	46.09%	11.193%
12	13.157	1707	1712	1720	rBV2	18720	27121	1.50%	0.365%
13	13.645	1789	1795	1801	rBV4	11645	22578	1.25%	0.304%
14	14.045	1857	1863	1872	rBV	48431	71823	3.98%	0.966%
15	14.322	1903	1910	1916	rBV	108043	156635	8.68%	2.107%
16	14.387	1916	1921	1930	rVB3	12264	22586	1.25%	0.304%
17	14.728	1972	1979	1985	rVB	50619	68914	3.82%	0.927%
18	15.375	2084	2089	2101	rVB	72504	113412	6.28%	1.526%
19	15.822	2154	2165	2179	rBV	636008	938640	52.00%	12.629%
20	16.898	2340	2348	2353	rBV	15460	27341	1.51%	0.368%
21	17.081	2372	2379	2382	rBV	151101	217880	12.07%	2.931%
22	17.122	2382	2386	2394	rVV	140577	195669	10.84%	2.633%
23	17.216	2394	2402	2408	rVV	20595	34857	1.93%	0.469%
24	17.498	2445	2450	2458	rVB	43155	63141	3.50%	0.850%
25	17.980	2529	2532	2535	rBV3	30008	38044	2.11%	0.512%
26	18.145	2555	2560	2565	rBV	30035	46776	2.59%	0.629%
27	18.245	2573	2577	2581	rBV2	13542	25036	1.39%	0.337%
28	19.063	2712	2716	2719	rBV3	15246	21975	1.22%	0.296%
29	19.104	2719	2723	2727	rVB	36227	48233	2.67%	0.649%
30	19.451	2779	2782	2787	rVB	35420	42500	2.35%	0.572%
31	19.657	2811	2817	2823	rBV	1588445	1804942	100.00%	24.284%
32	19.775	2832	2837	2839	rBV2	26944	37646	2.09%	0.506%
33	19.833	2844	2847	2850	rVV	24414	29086	1.61%	0.391%
34	19.910	2857	2860	2869	rVB2	22427	35336	1.96%	0.475%
35	20.510	2958	2962	2966	rBV3	20229	29820	1.65%	0.401%
36	20.551	2967	2969	2976	rVB5	14544	19570	1.08%	0.263%

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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

37	20.904	3025	3029	3035	rVB2	45578	71945	3.99%	0.968%
38	20.963	3035	3039	3045	rBV	39808	50407	2.79%	0.678%
39	21.180	3071	3076	3086	rBV	263563	329661	18.26%	4.435%
40	21.680	3158	3161	3166	rBV2	21203	31590	1.75%	0.425%
41	23.480	3461	3467	3475	rVB	180350	331462	18.36%	4.460%

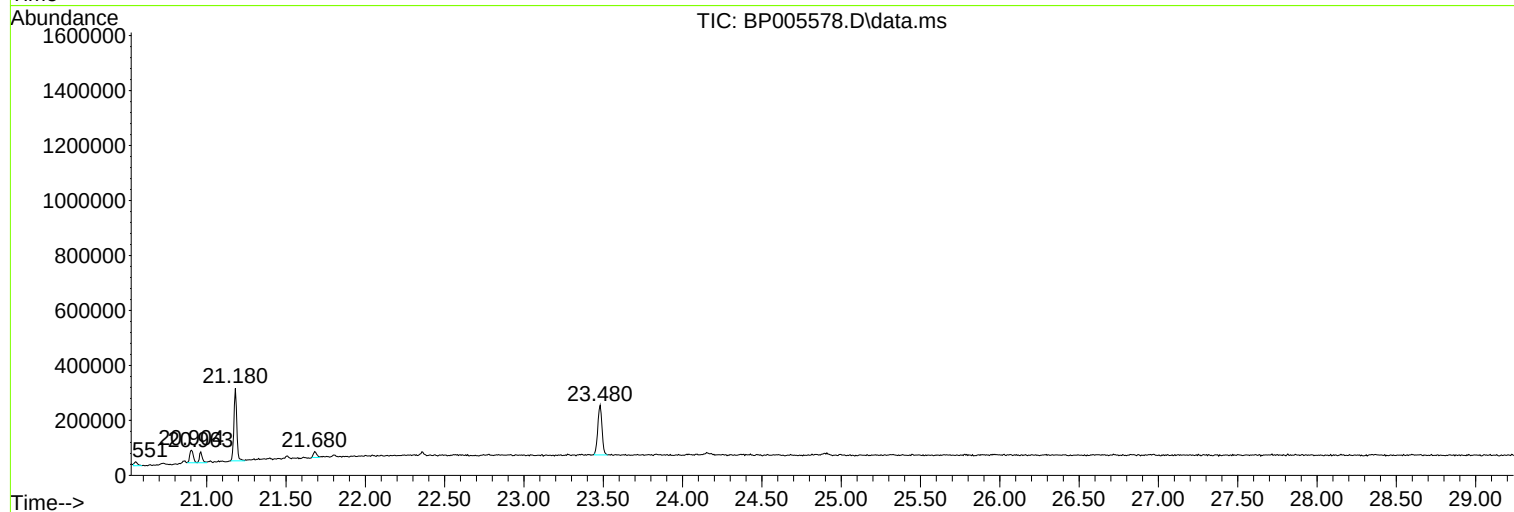
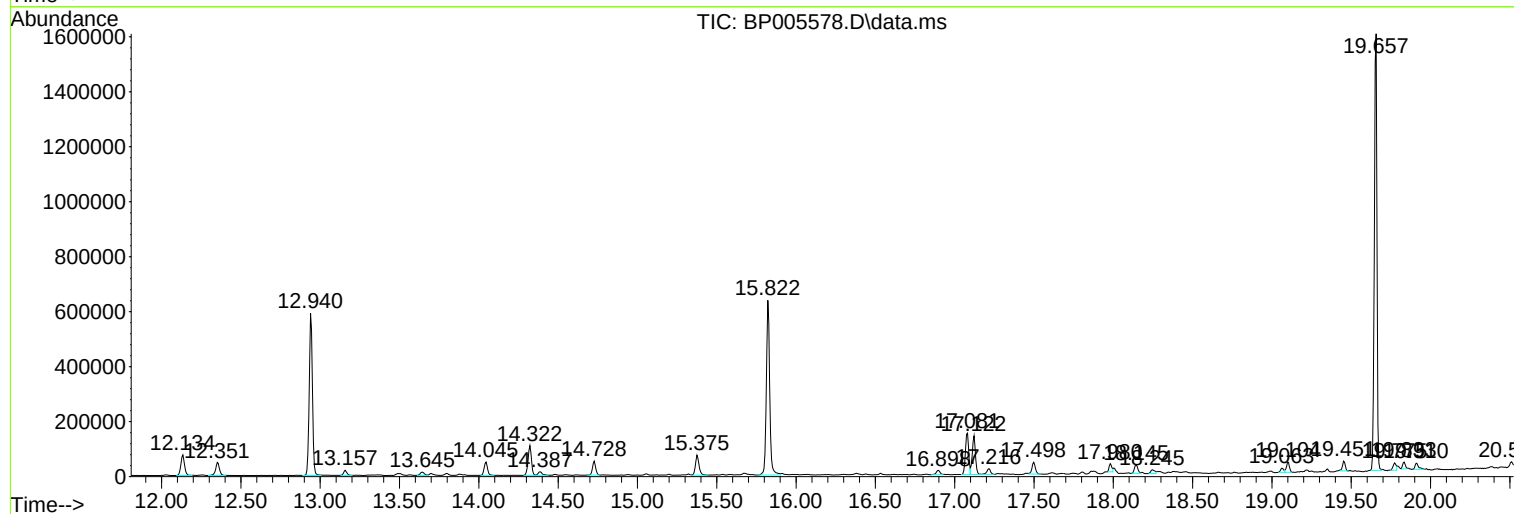
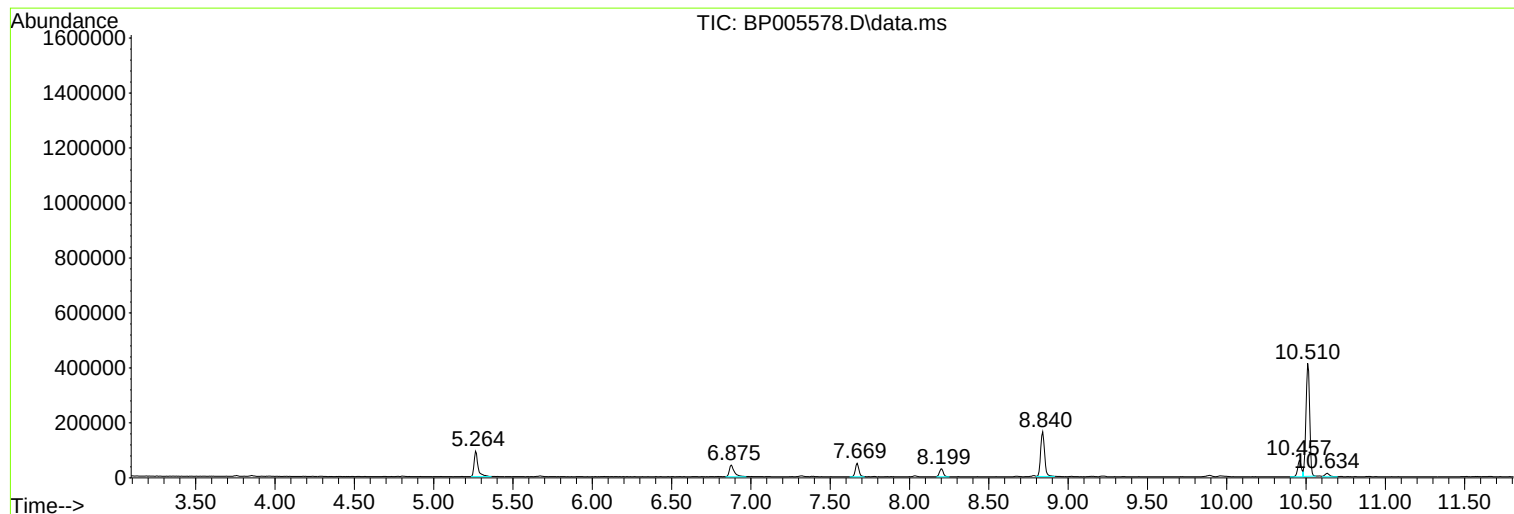
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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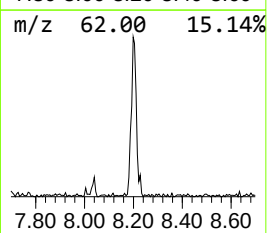
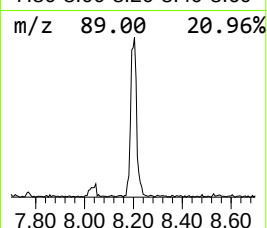
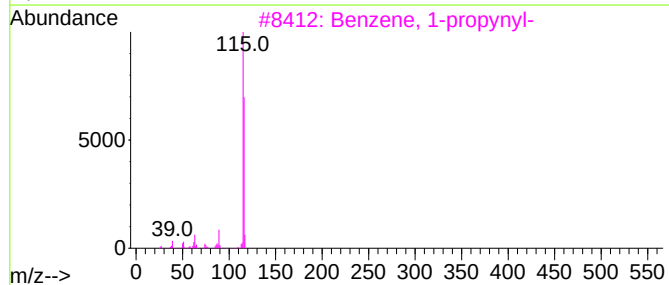
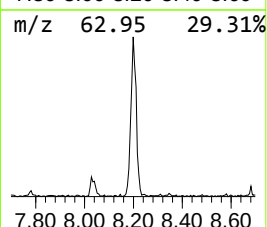
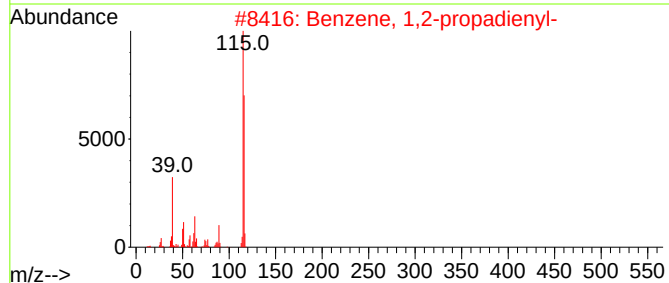
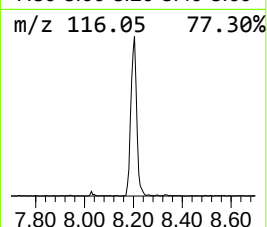
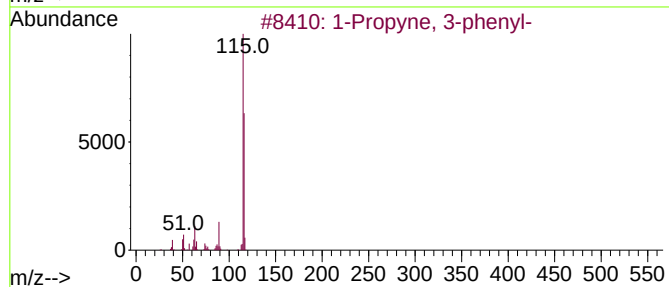
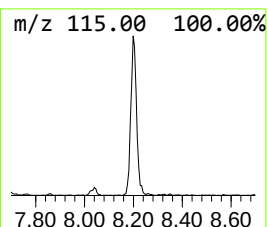
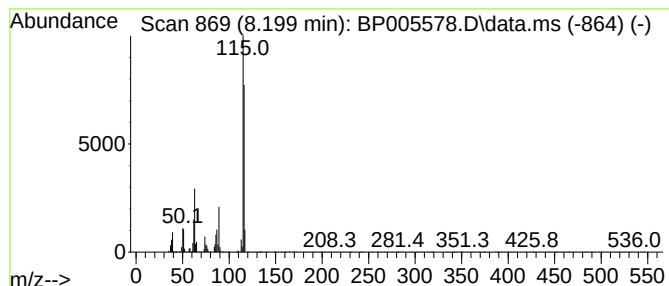
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Propyne, 3-phenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.199	12.77 ng	49487	1,4-Dichlorobenzene-d4	7.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	91
2			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
3			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
4			2-Methylphenylacetylene	116	C9H8	000766-47-2	90
5			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	87



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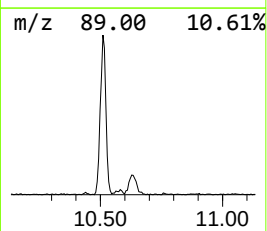
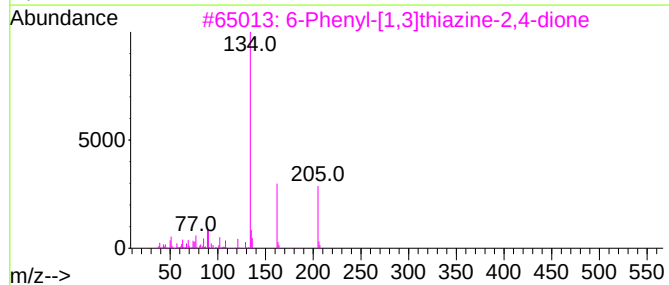
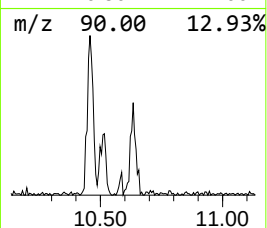
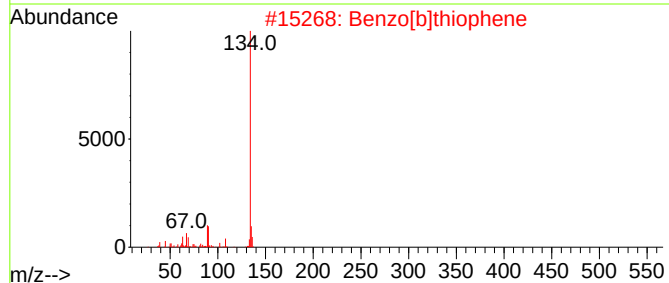
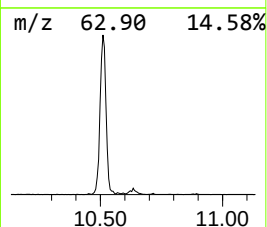
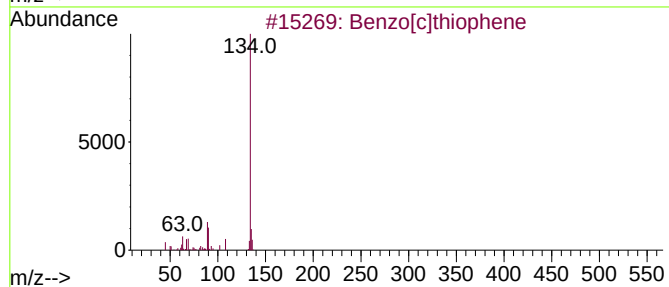
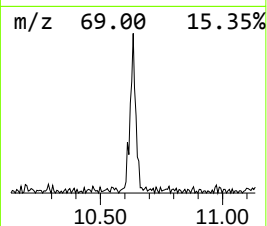
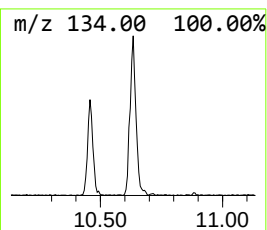
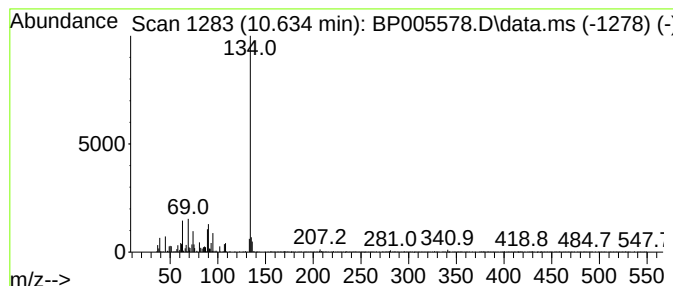
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzo[c]thiophene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	4.58 ng	23452	Naphthalene-d8	10.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[c]thiophene	134	C8H6S	000270-82-6	87
2			Benzo[b]thiophene	134	C8H6S	000095-15-8	83
3			6-Phenyl-[1,3]thiazine-2,4-dione	205	C10H7N02S	1000300-90-1	56
4			Furan-2-carboxylic acid, 5-cyano...	165	C8H7NO3	1000303-92-6	40
5			Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	40



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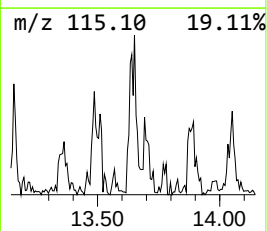
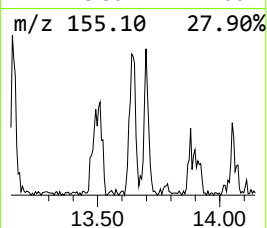
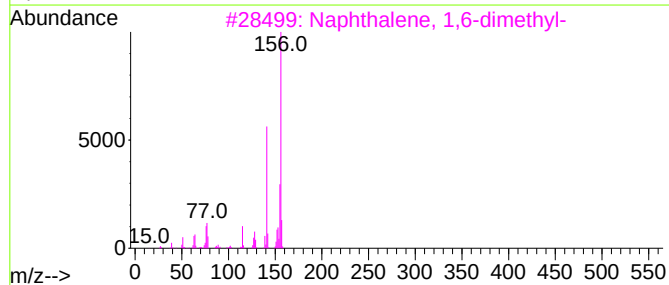
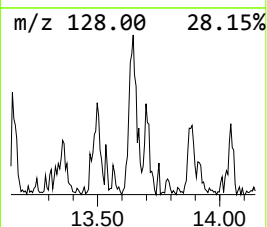
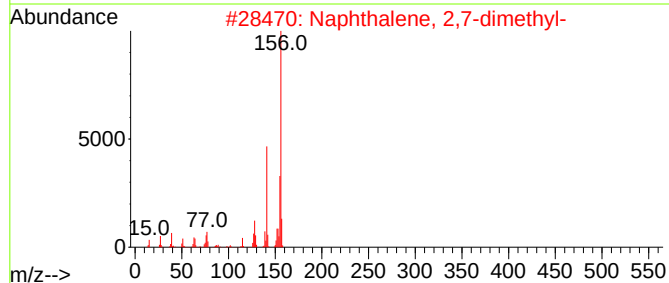
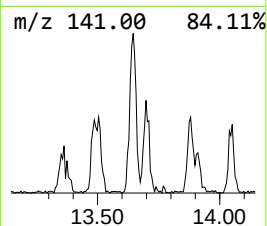
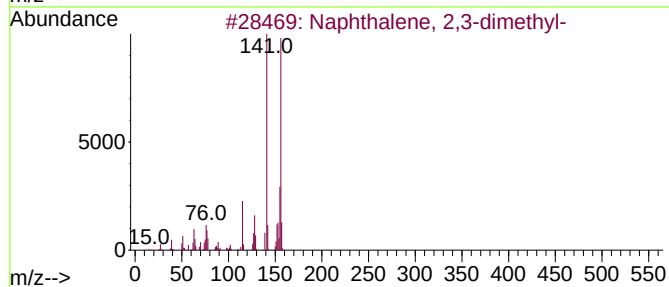
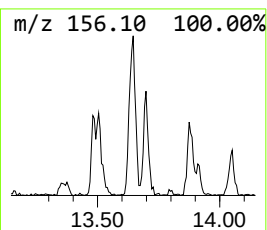
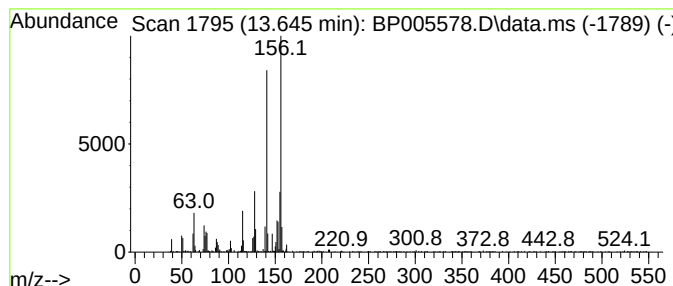
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.645	2.88 ng	22578	Acenaphthene-d10	14.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	93
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	91
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	91
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	91



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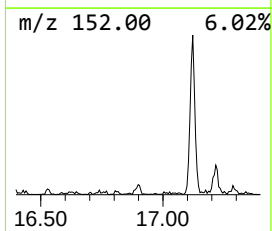
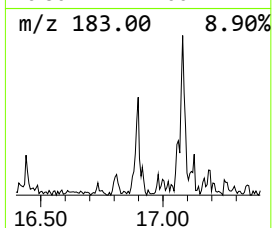
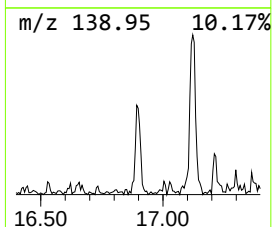
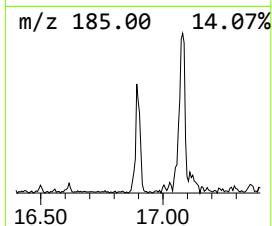
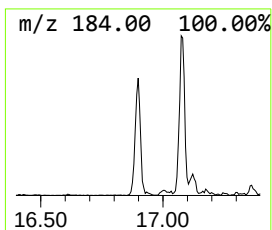
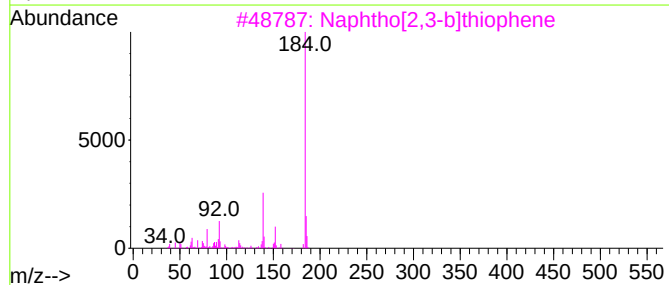
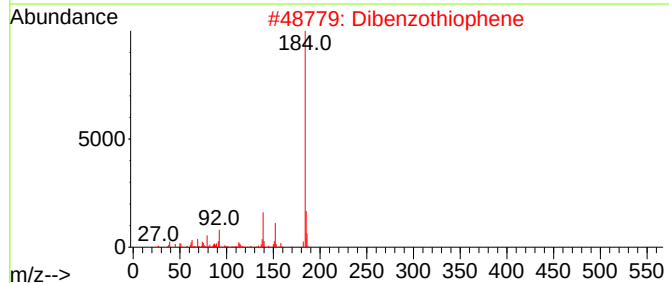
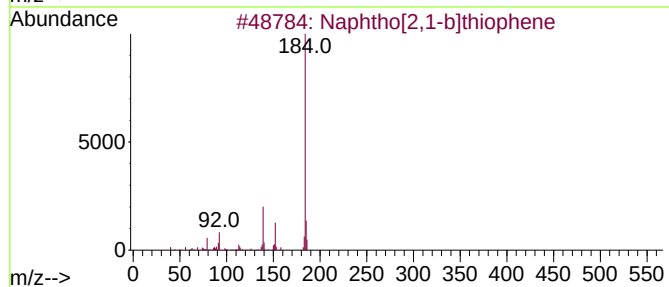
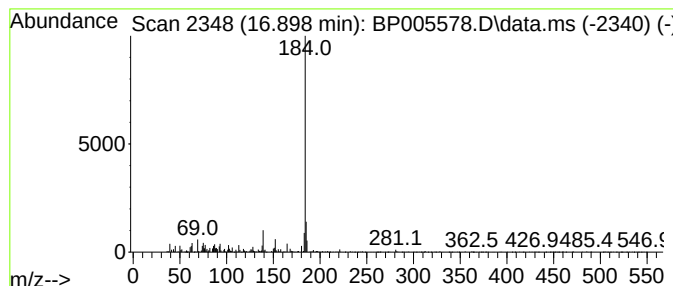
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphtho[2,1-b]thiophene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.898	2.51 ng	27341	Phenanthrene-d10	17.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphtho[2,1-b]thiophene	184	C12H8S	000233-02-3	90
2			Dibenzothiophene	184	C12H8S	000132-65-0	87
3			Naphtho[2,3-b]thiophene	184	C12H8S	000268-77-9	83
4			Naphtho[1,2-b]thiophene	184	C12H8S	000234-41-3	83
5			Azuleno(2,1-b)thiophene	184	C12H8S	000248-13-5	78



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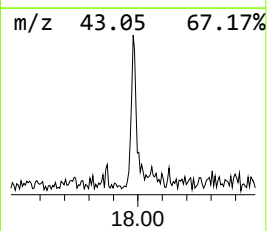
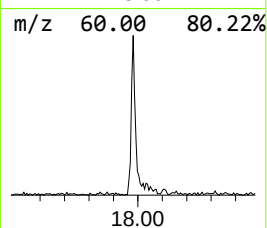
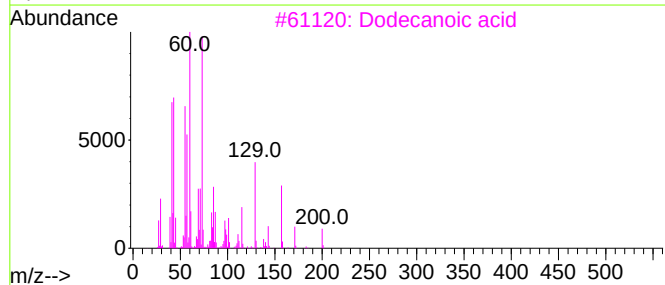
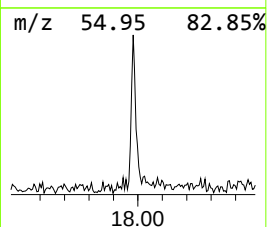
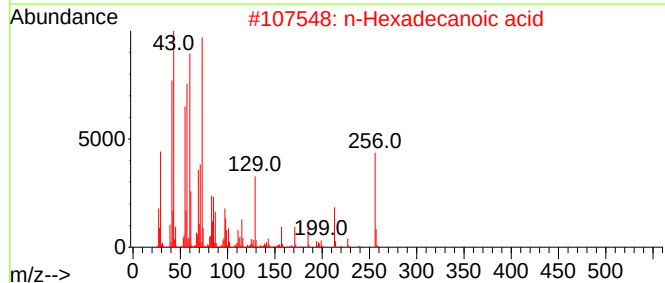
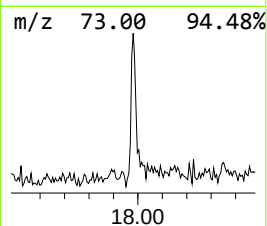
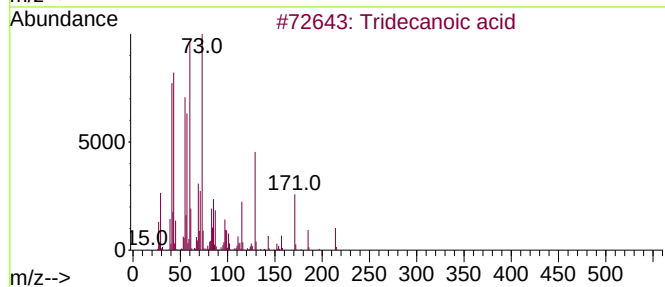
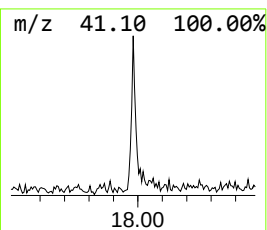
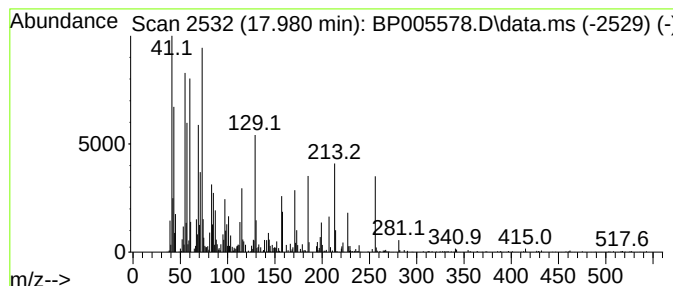
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	3.49 ng	38044	Phenanthrene-d10	17.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3			Dodecanoic acid	200	C12H24O2	000143-07-7	50
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
Data File : BP005578.D
Acq On : 15 May 2021 20:36
Operator : CG/JU
Sample : M2383-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DUP-02-05122021

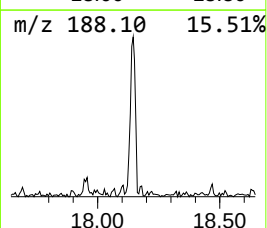
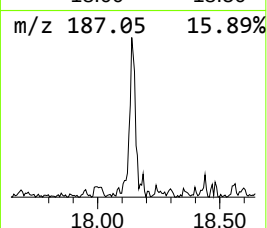
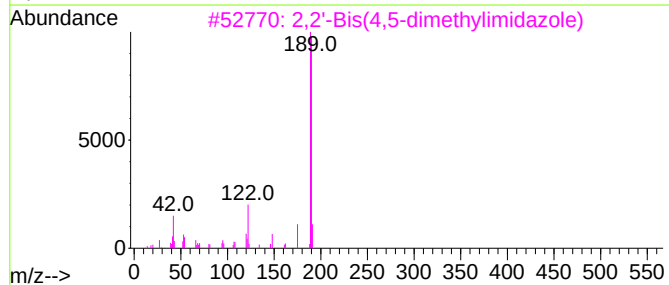
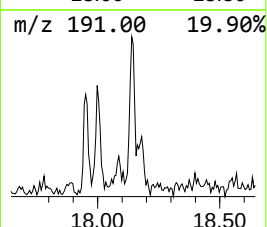
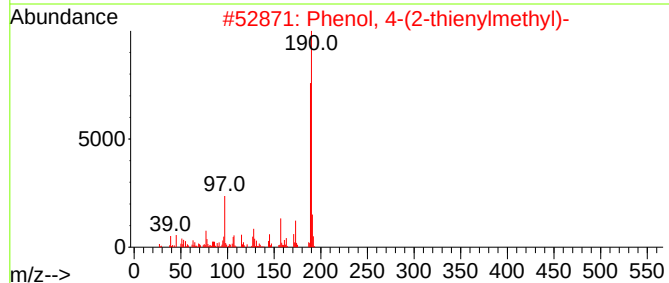
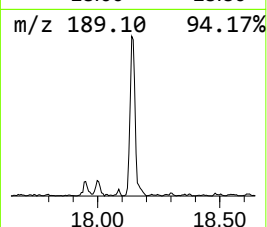
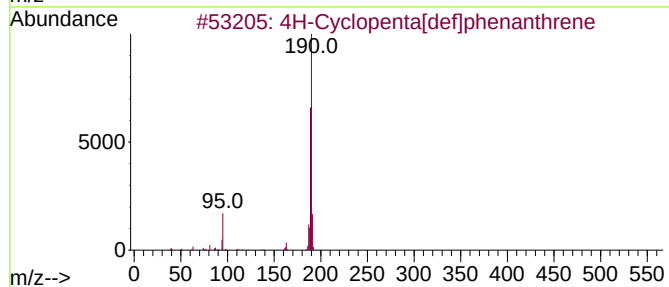
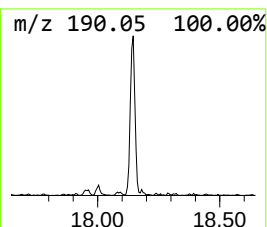
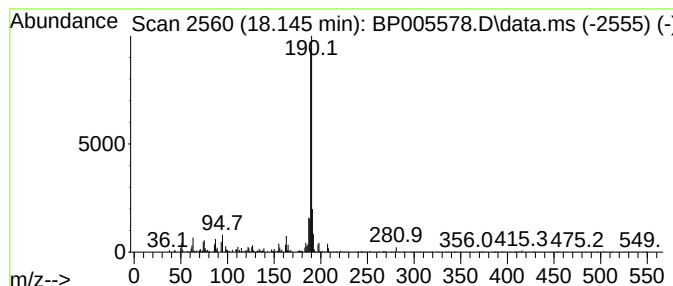
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	4.29 ng	46776	Phenanthrene-d10	17.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2			Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	72
3			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	59
4			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	56
5			8H-Imidazo[4,5-E]-2,1,3-benzothi...	190	C8H6N4S	129485-68-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
Data File : BP005578.D
Acq On : 15 May 2021 20:36
Operator : CG/JU
Sample : M2383-12
Misc :
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ClientSampleId :
DUP-02-05122021

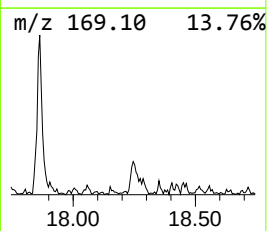
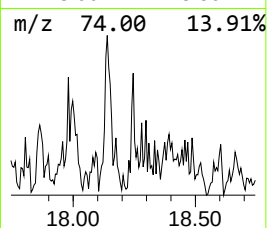
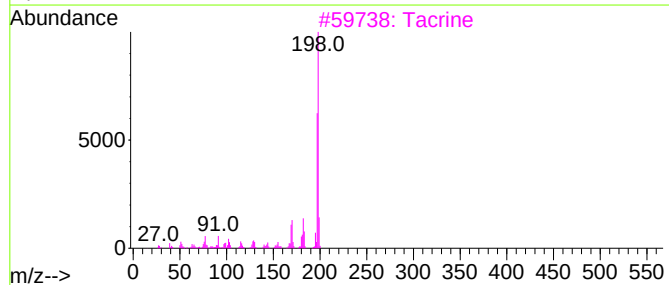
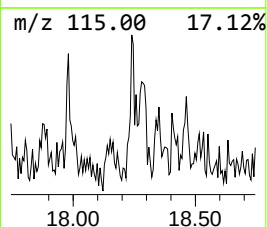
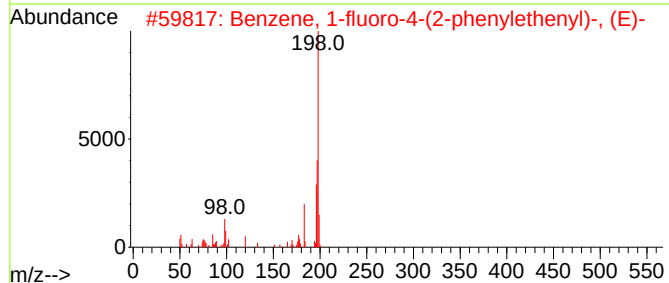
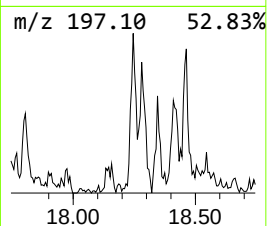
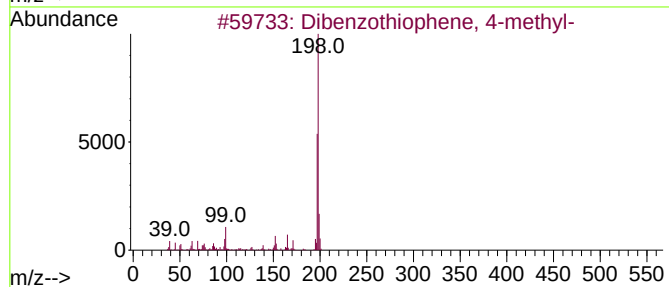
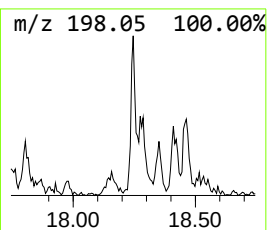
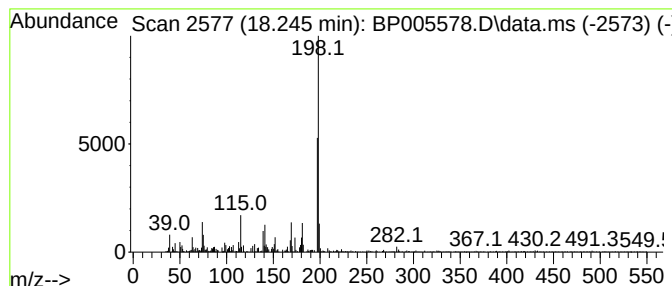
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dibenzothiophene, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	2.30 ng	25036	Phenanthrene-d10	17.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzothiophene, 4-methyl-	198	C13H10S	007372-88-5	80
2			Benzene, 1-fluoro-4-(2-phenyleth...	198	C14H11F	000718-25-2	72
3			Tacrine	198	C13H14N2	000321-64-2	72
4			Benzenamine, 4,4'-methylenebis-	198	C13H14N2	000101-77-9	72
5			Benzene, 1-fluoro-4-(2-phenyleth...	198	C14H11F	017404-69-2	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
Data File : BP005578.D
Acq On : 15 May 2021 20:36
Operator : CG/JU
Sample : M2383-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

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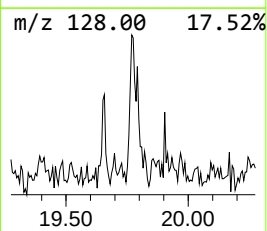
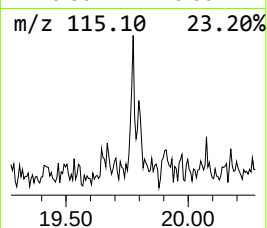
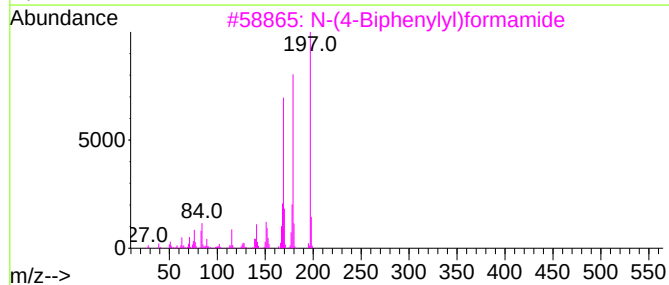
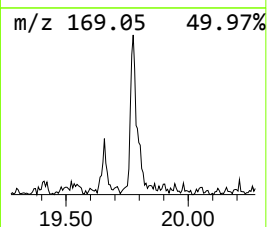
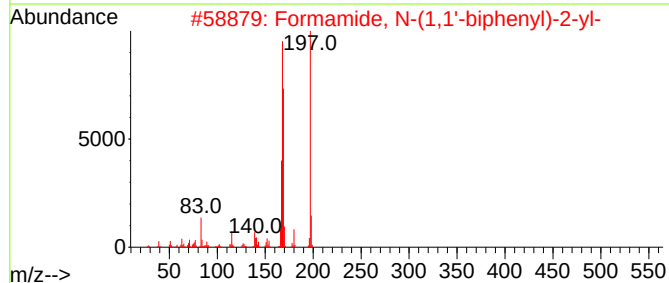
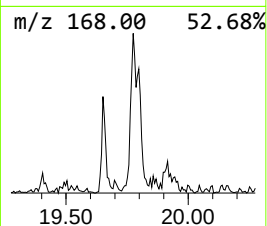
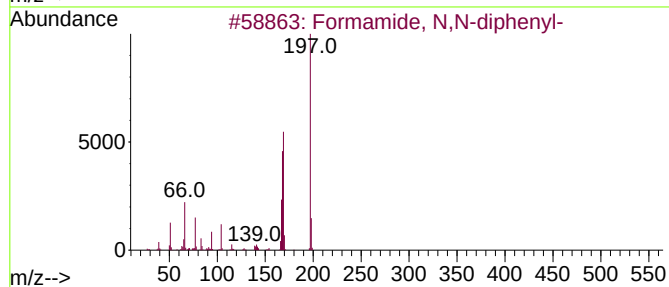
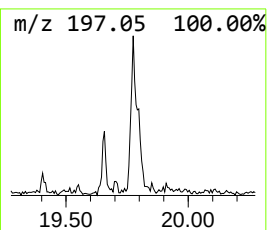
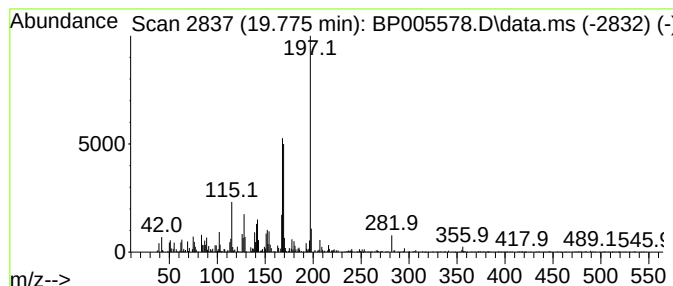
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Formamide, N,N-diphenyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.775	2.28 ng	37646	Chrysene-d12	21.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N,N-diphenyl-	197	C13H11NO	000607-00-1	64
2			Formamide, N-(1,1'-biphenyl)-2-yl-	197	C13H11NO	005346-21-4	64
3			N-(4-Biphenyl)formamide	197	C13H11NO	005472-79-7	58
4			1,5-Diacetylnaphthalene	212	C14H12O2	003027-43-8	53
5			1-Ethanone, 1-[4-amino-2-(2-prop...	197	C8H11N3OS	1000338-04-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
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Acq On : 15 May 2021 20:36
Operator : CG/JU
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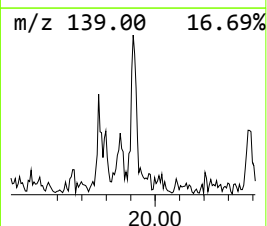
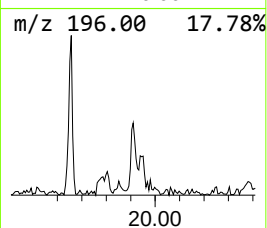
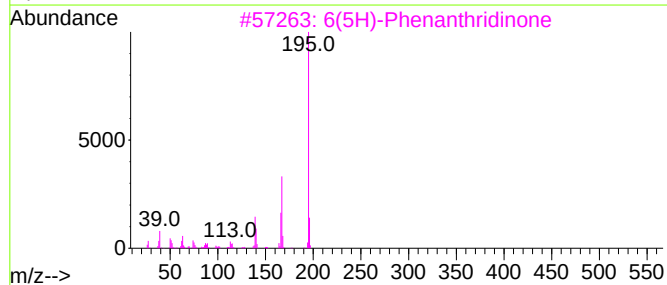
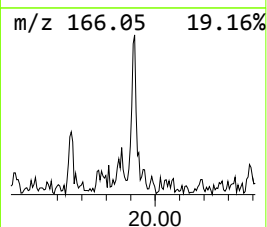
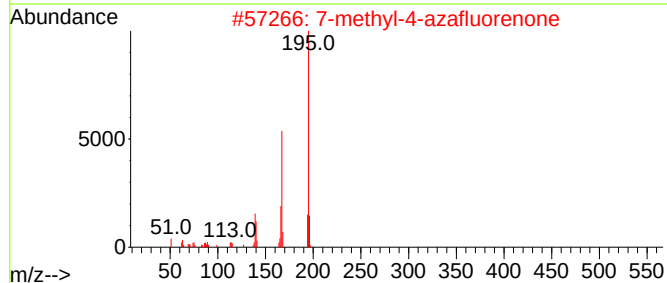
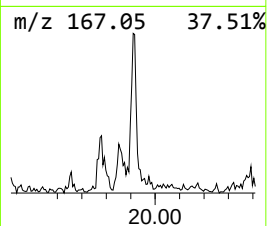
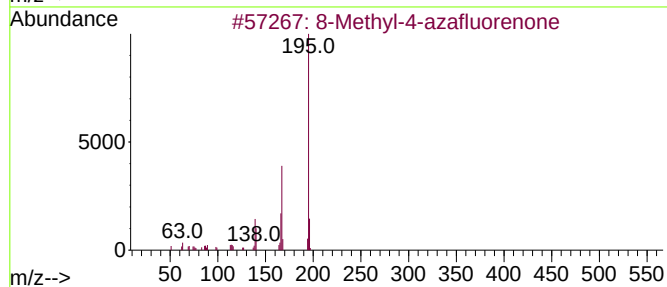
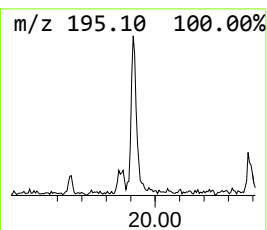
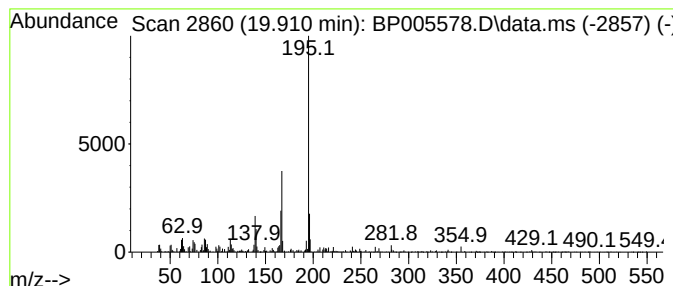
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 8-Methyl-4-azafluorenone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.910	2.14 ng	35336	Chrysene-d12		21.180	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	8-Methyl-4-azafluorenone		195	C13H9NO	064292-03-1	93
2	7-methyl-4-azafluorenone		195	C13H9NO	064292-02-0	93
3	6(5H)-Phenanthridinone		195	C13H9NO	001015-89-0	93
4	4-Amino-9-fluorenone		195	C13H9NO	004269-15-2	90
5	Benzo[c]cinnolin-2-amine		195	C12H9N3	004827-07-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
Data File : BP005578.D
Acq On : 15 May 2021 20:36
Operator : CG/JU
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP-02-05122021

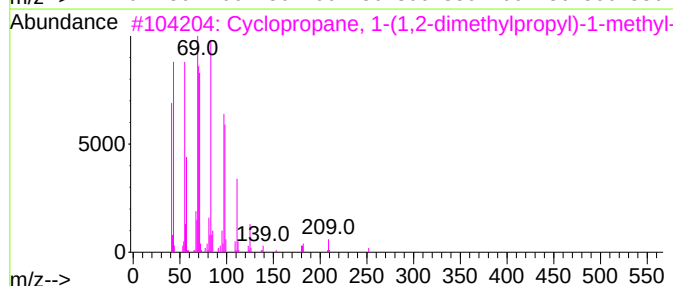
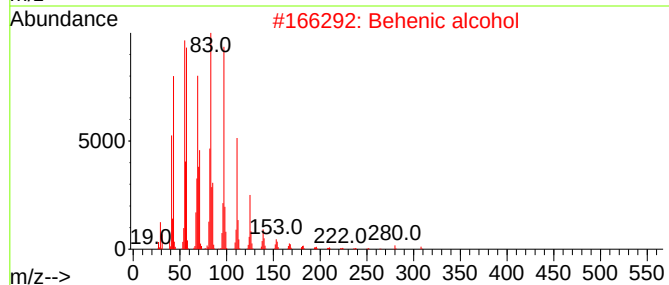
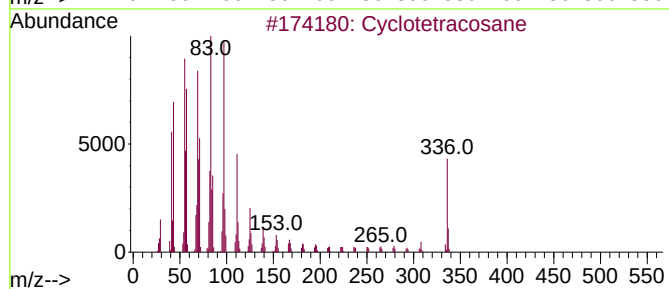
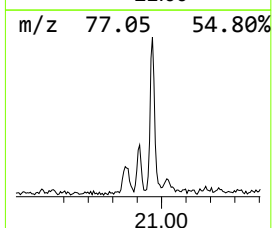
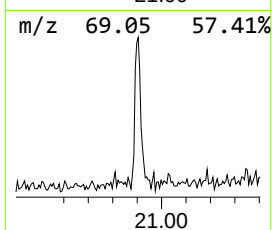
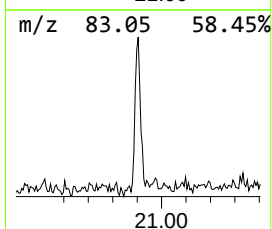
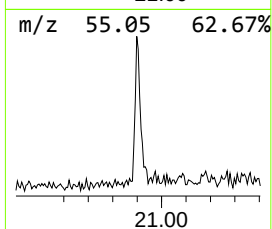
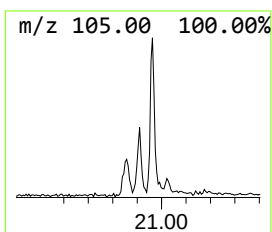
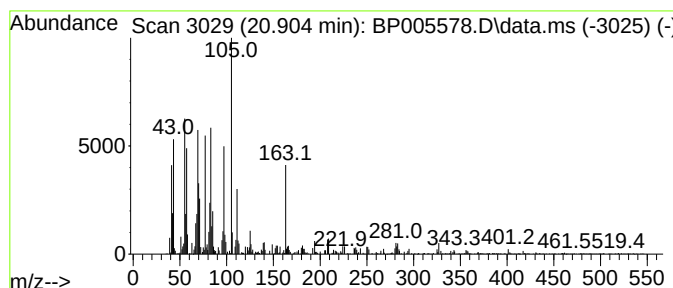
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclotetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.904	4.36 ng	71945	Chrysene-d12	21.180

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	89
2		Behenic alcohol	326	C22H46O	000661-19-8	55
3		Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	50
4		E-15-Heptadecenal	252	C17H32O	1000130-97-9	49
5		Octacosyl acetate	452	C30H60O2	018206-97-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
Data File : BP005578.D
Acq On : 15 May 2021 20:36
Operator : CG/JU
Sample : M2383-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DUP-02-05122021

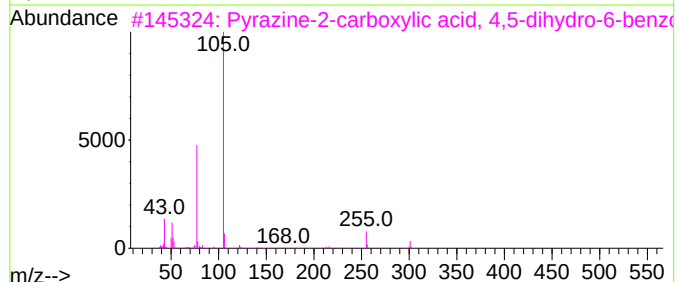
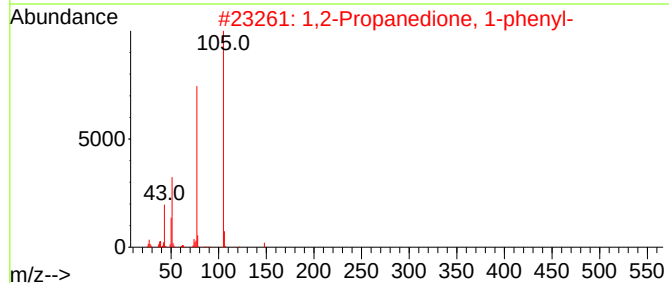
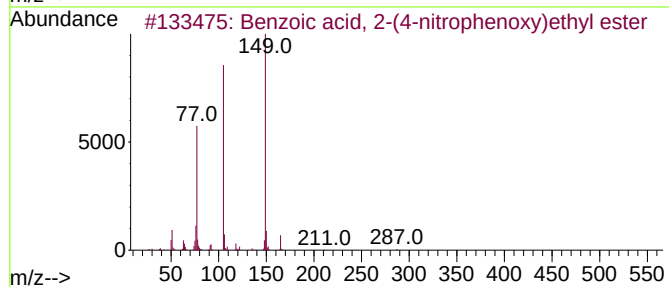
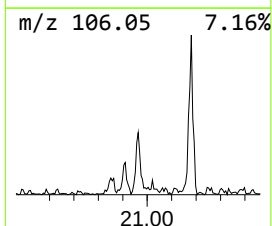
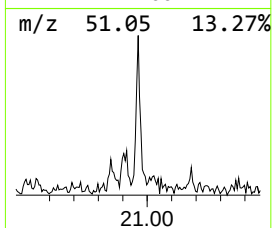
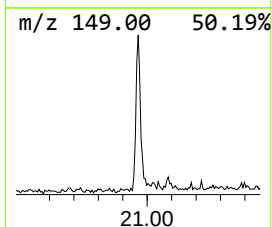
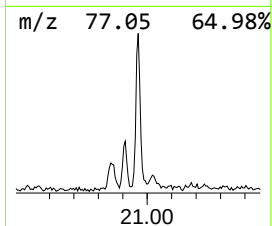
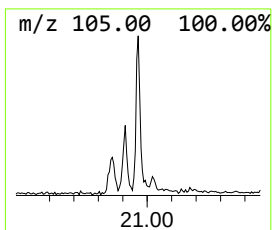
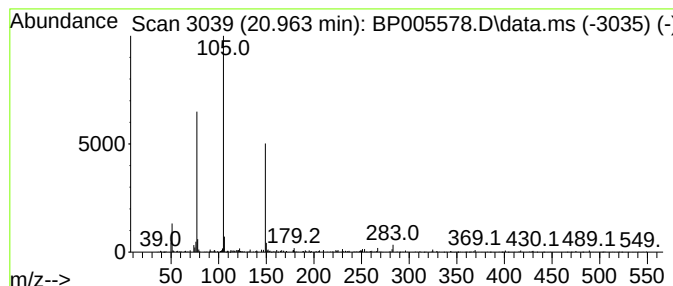
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzoic acid, 2-(4-nitrophe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.963	3.06 ng	50407	Chrysene-d12	21.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	50
2			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	38
3			Pyrazine-2-carboxylic acid, 4,5-...	301	C15H15N3O4	1000259-49-5	38
4			2-Chloro-1,4-dibenzamido benzene	350	C20H15ClN2O2	300360-38-7	38
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051521\
Data File : BP005578.D
Acq On : 15 May 2021 20:36
Operator : CG/JU
Sample : M2383-12
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propyne, 3-ph...	8.199	12.8	ng	49487	1	7.669	77534	20.0
Benzo[c]thiophene	10.634	4.6	ng	23452	2	10.463	102305	20.0
Naphthalene, 2,...	13.645	2.9	ng	22578	3	14.322	156635	20.0
Naphtho[2,1-b]t...	16.898	2.5	ng	27341	4	17.081	217880	20.0
Tridecanoic acid	17.980	3.5	ng	38044	4	17.081	217880	20.0
4H-Cyclopenta[d...	18.145	4.3	ng	46776	4	17.081	217880	20.0
Dibenzothiophen...	18.245	2.3	ng	25036	4	17.081	217880	20.0
Formamide, N,N-...	19.775	2.3	ng	37646	5	21.180	329661	20.0
8-Methyl-4-azaf...	19.910	2.1	ng	35336	5	21.180	329661	20.0
Cyclotetracosane	20.904	4.4	ng	71945	5	21.180	329661	20.0
Benzoic acid, 2...	20.963	3.1	ng	50407	5	21.180	329661	20.0