

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
 Data File : BP005268.D
 Acq On : 12 Apr 2021 16:17
 Operator : CG/JU
 Sample : M1967-11
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB1-C

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-BP040921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.816	291	294	304	rVB	263499	389568	26.08%	4.231%
2	5.281	368	373	381	rVB	397787	584426	39.13%	6.347%
3	6.863	636	642	644	rBV	510431	773589	51.79%	8.402%
4	6.893	644	647	659	rVB	518799	780395	52.25%	8.476%
5	7.675	774	780	787	rBV	131350	206455	13.82%	2.242%
6	7.746	787	792	798	rVB3	13956	21810	1.46%	0.237%
7	8.840	970	978	986	rBV	319510	512343	34.30%	5.565%
8	10.463	1245	1254	1260	rBV	146094	247643	16.58%	2.690%
9	11.981	1506	1512	1519	rBV2	34341	62048	4.15%	0.674%
10	12.951	1668	1677	1691	rBV	652005	924842	61.92%	10.045%
11	13.798	1816	1821	1829	rBV3	17414	32759	2.19%	0.356%
12	14.339	1906	1913	1921	rBV	219132	317947	21.29%	3.453%
13	14.939	2003	2015	2017	rBV4	15446	51096	3.42%	0.555%
14	15.839	2163	2168	2174	rBV3	39348	60230	4.03%	0.654%
15	16.086	2204	2210	2215	rBV4	16572	28930	1.94%	0.314%
16	16.498	2276	2280	2288	rVB9	8968	18244	1.22%	0.198%
17	16.916	2349	2351	2360	rVB6	12321	17748	1.19%	0.193%
18	17.104	2377	2383	2387	rBV	281400	407658	27.29%	4.428%
19	17.145	2387	2390	2394	rVV	29545	41707	2.79%	0.453%
20	17.198	2395	2399	2402	rVV	34155	45184	3.03%	0.491%
21	17.227	2402	2404	2410	rVB4	24176	35485	2.38%	0.385%
22	17.998	2533	2535	2539	rBV5	10411	14972	1.00%	0.163%
23	18.151	2557	2561	2567	rVB4	26544	42032	2.81%	0.457%
24	18.992	2700	2704	2713	rVB	46008	78148	5.23%	0.849%
25	19.127	2723	2727	2733	rVB	66629	84742	5.67%	0.920%
26	19.186	2733	2737	2740	rBV5	13747	19392	1.30%	0.211%
27	19.480	2783	2787	2789	rBV	53666	65734	4.40%	0.714%
28	19.680	2816	2821	2828	rVB	1292937	1493647	100.00%	16.222%
29	20.510	2959	2962	2966	rBV	50561	62130	4.16%	0.675%
30	20.886	3021	3026	3028	rBV2	64540	98964	6.63%	1.075%
31	20.933	3028	3034	3039	rVV2	133016	298006	19.95%	3.237%
32	20.986	3039	3043	3052	rVB	252469	331662	22.20%	3.602%
33	21.115	3062	3065	3071	rVB	53786	63913	4.28%	0.694%
34	21.204	3075	3080	3084	rBV	413161	542961	36.35%	5.897%
35	23.474	3461	3466	3473	rVB2	244137	450927	30.19%	4.897%

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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-BP040921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

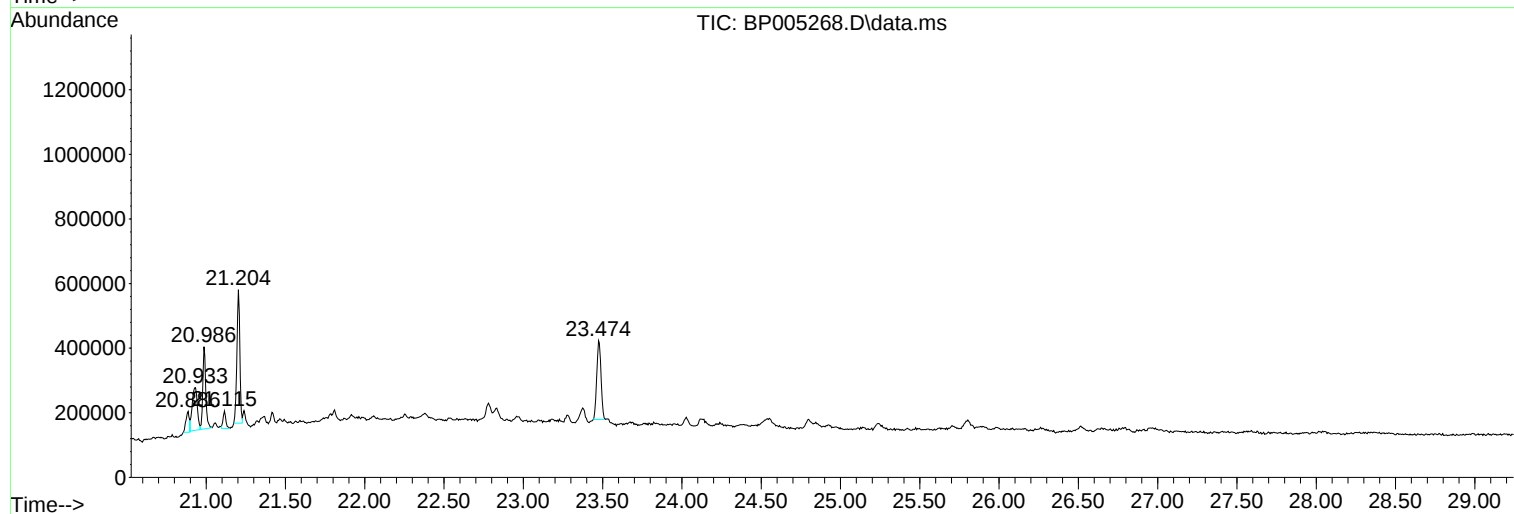
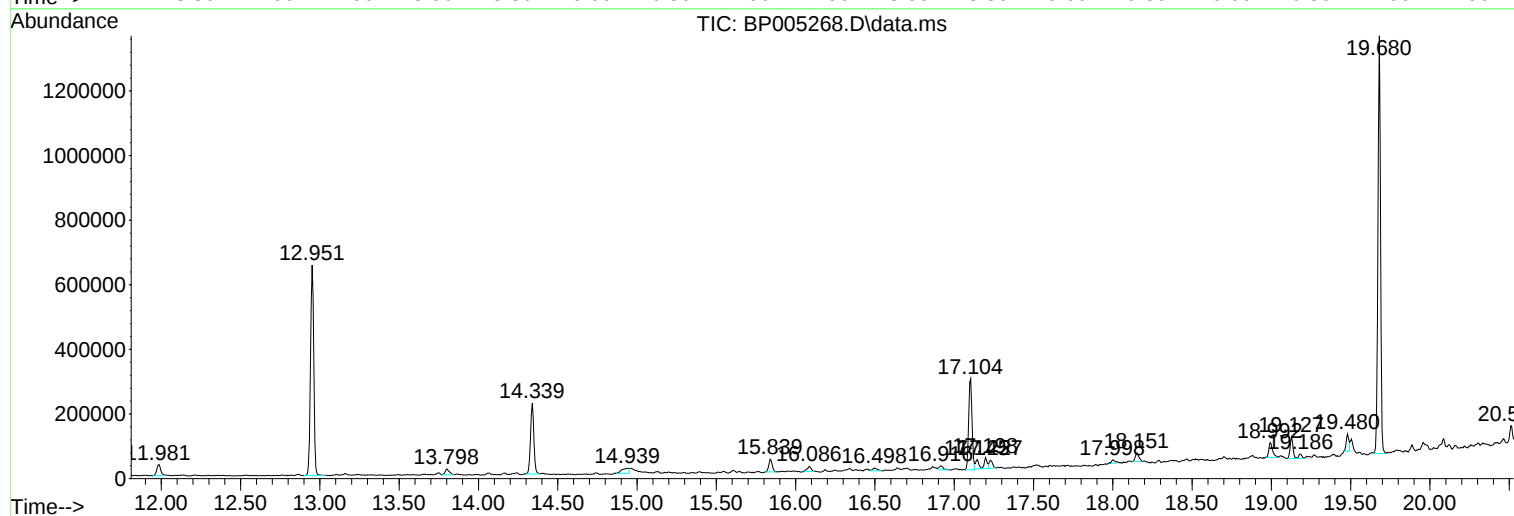
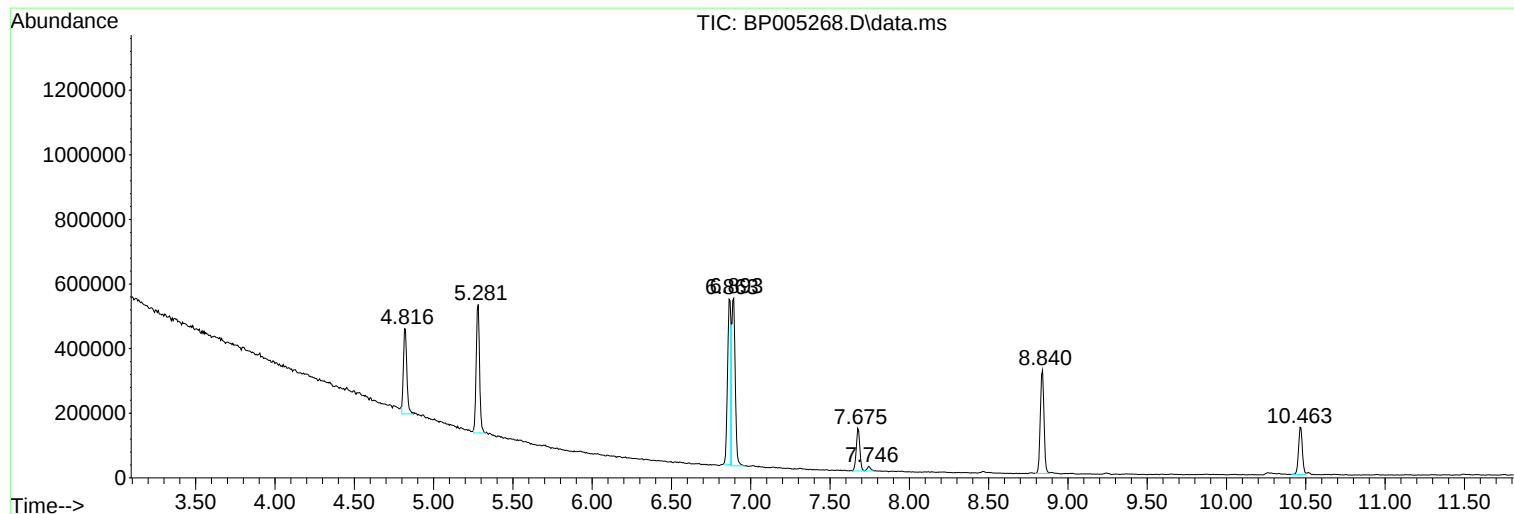
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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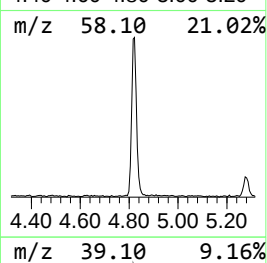
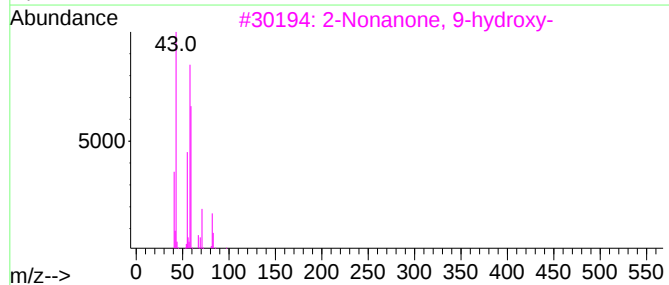
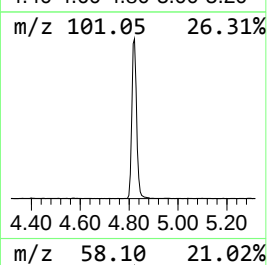
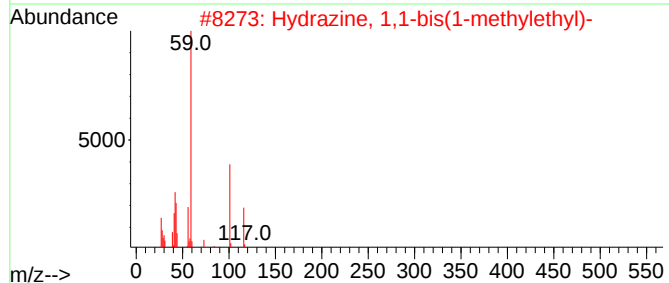
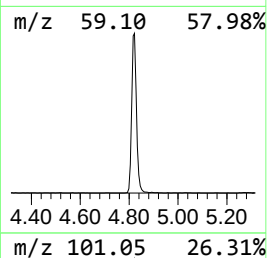
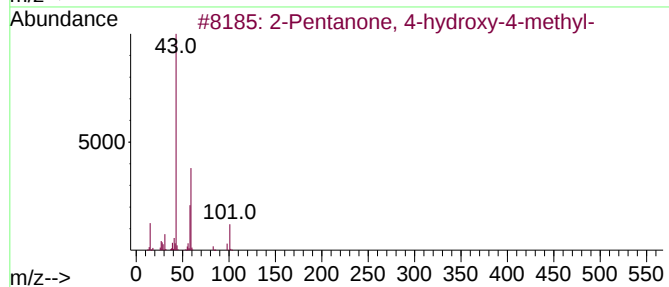
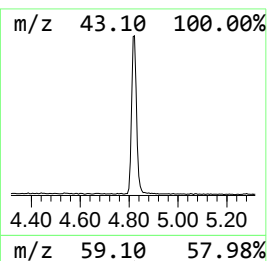
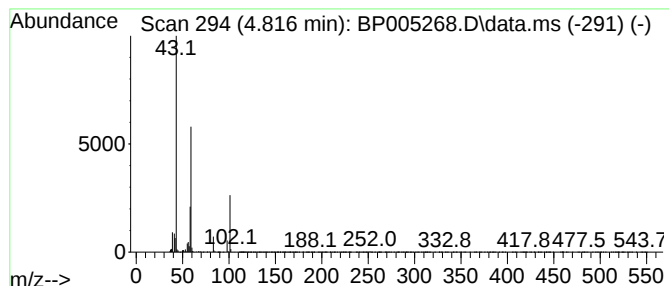
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.816	37.74 ng	389568	1,4-Dichlorobenzene-d4	7.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25		
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25		
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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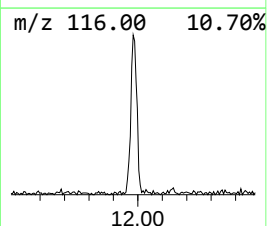
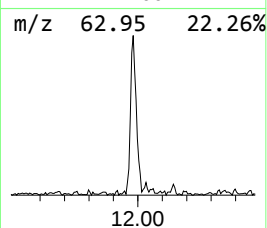
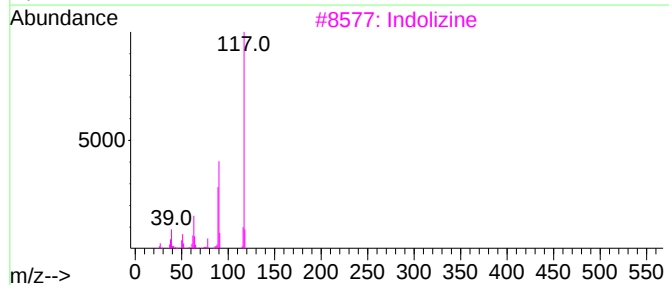
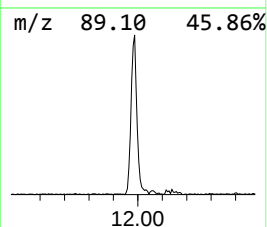
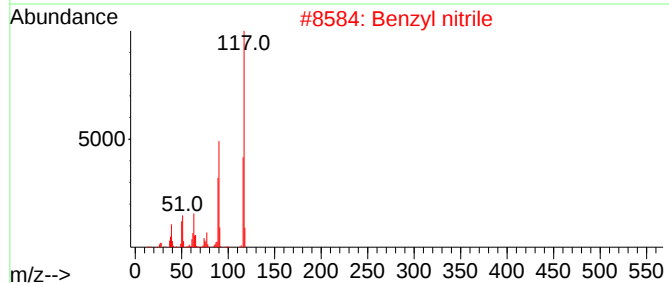
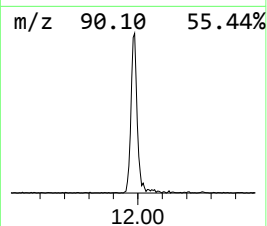
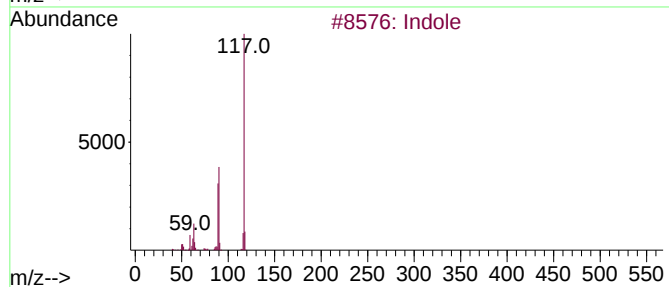
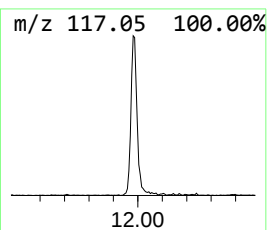
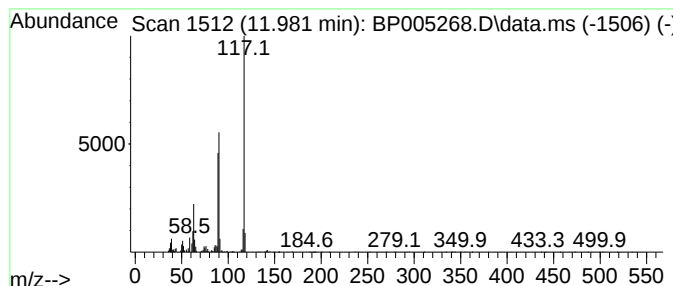
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Indole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.981	5.01 ng	62048	Naphthalene-d8	10.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	95
2			Benzyl nitrile	117	C8H7N	000140-29-4	91
3			Indolizine	117	C8H7N	000274-40-8	91
4			Benzonitrile, 2-methyl-	117	C8H7N	000529-19-1	90
5			5H-1-Pyridine	117	C8H7N	000270-91-7	87



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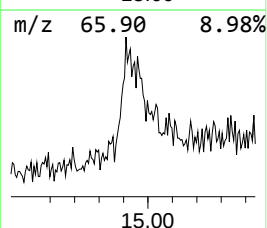
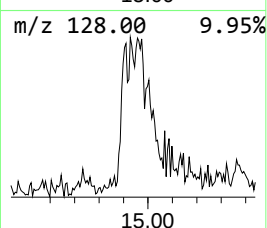
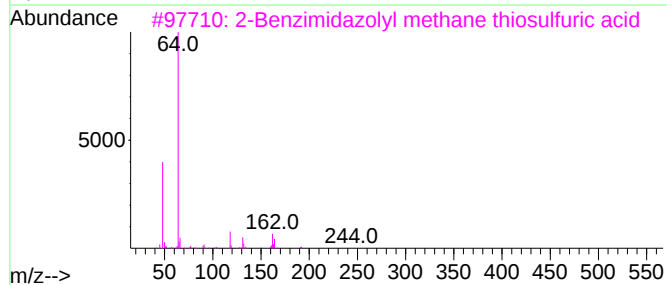
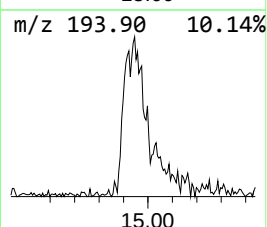
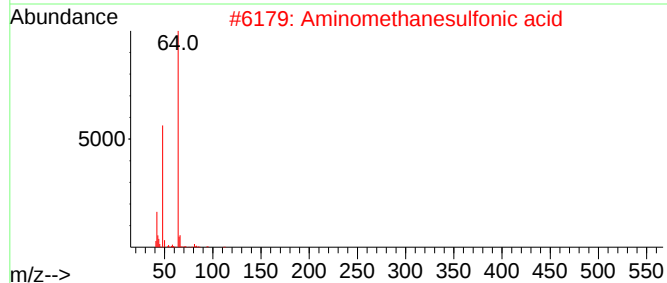
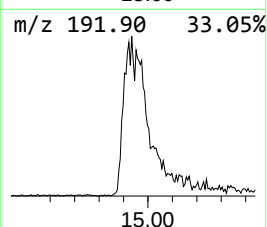
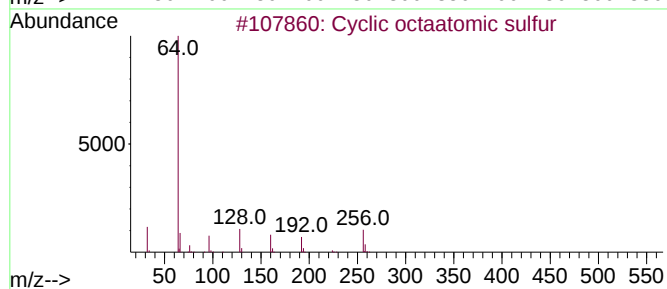
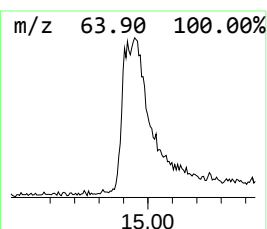
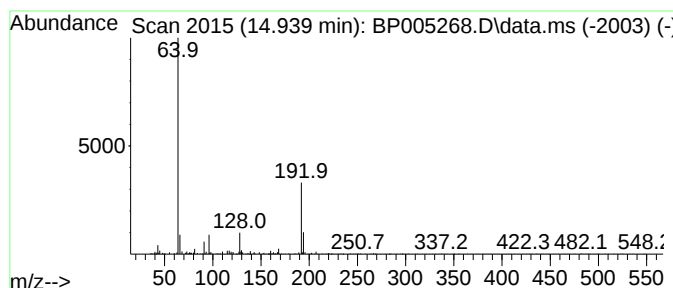
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.93 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.939	3.21 ng	51096	Acenaphthene-d10	14.339	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclic octaatomic sulfur	256	S8	010544-50-0	43
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3	2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1000256-39-2	5
4	Sulfur dioxide	64	O2S	007446-09-5	4
5	S-2-[3-Succinimidopropylamino]et...	296	C9H16N2O5S2	031701-75-4	4



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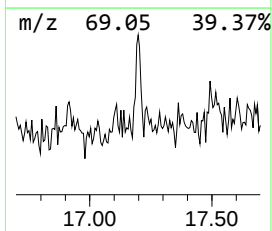
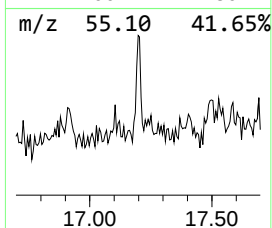
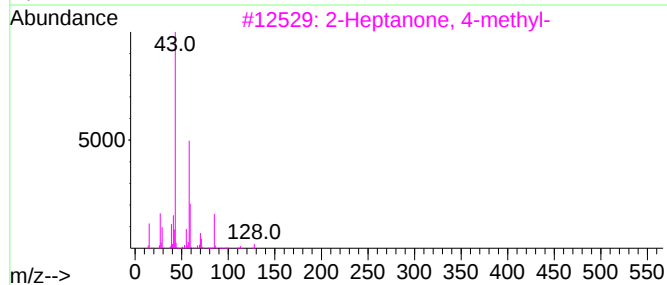
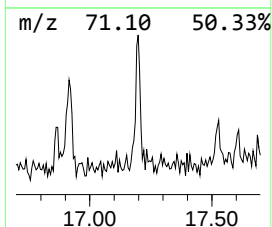
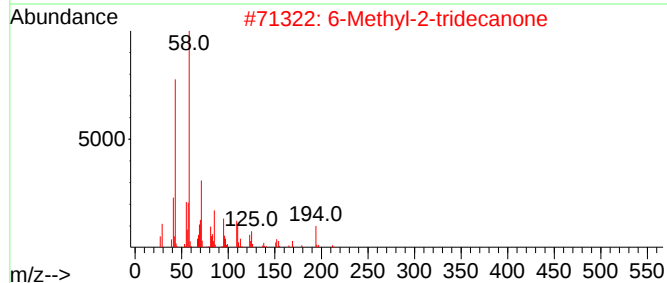
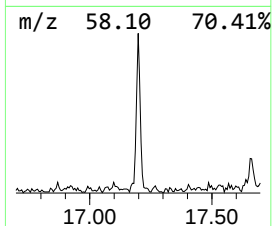
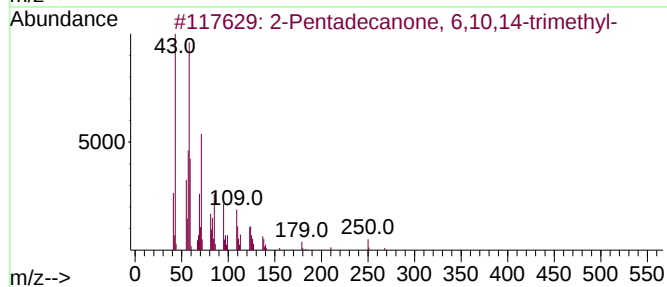
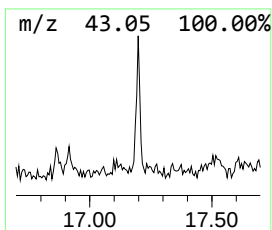
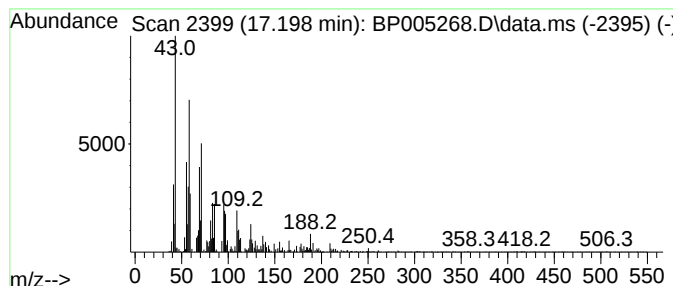
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentadecanone, 6,10,14-tr... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.198	2.22 ng	45184	Phenanthrene-d10		17.104	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentadecanone, 6,10,14-trimethyl-		268	C18H36O	000502-69-2	59
2	6-Methyl-2-tridecanone		212	C14H28O	073105-73-4	43
3	2-Heptanone, 4-methyl-		128	C8H16O	006137-06-0	38
4	2-Hexanone, 4-methyl-		114	C7H14O	000105-42-0	35
5	2-Dodecanone		184	C12H24O	006175-49-1	35



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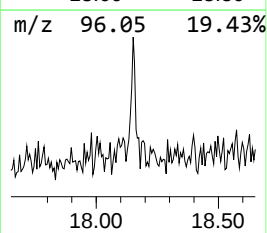
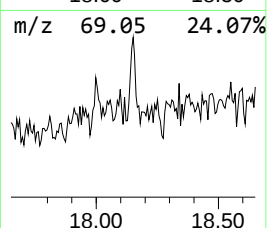
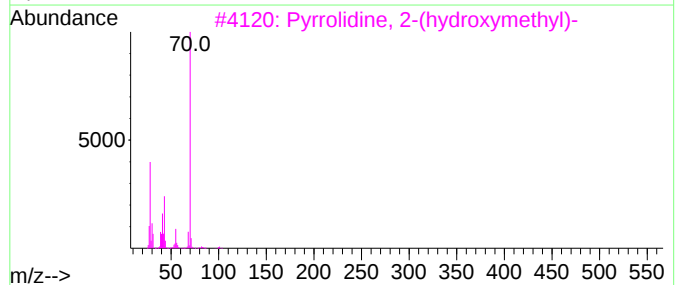
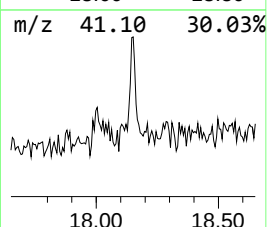
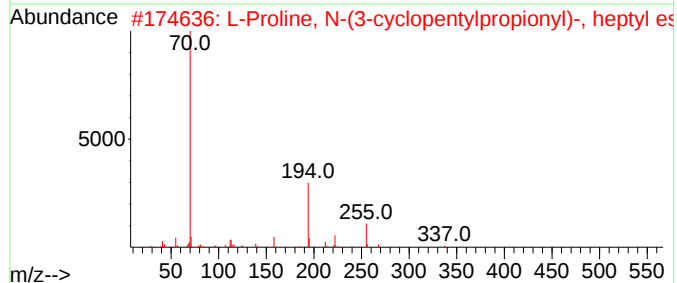
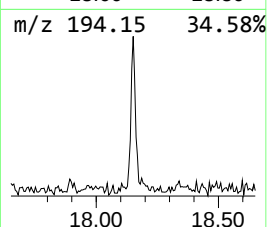
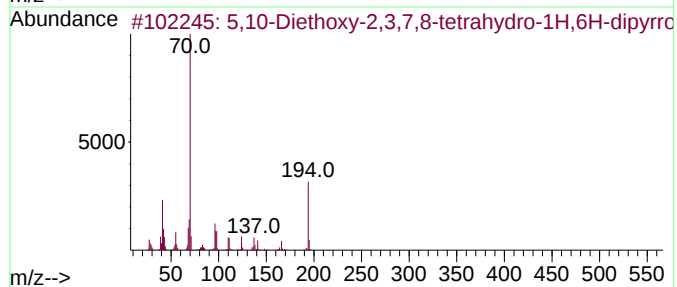
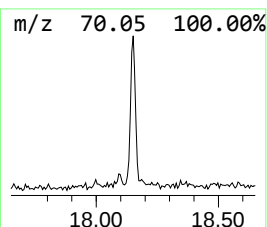
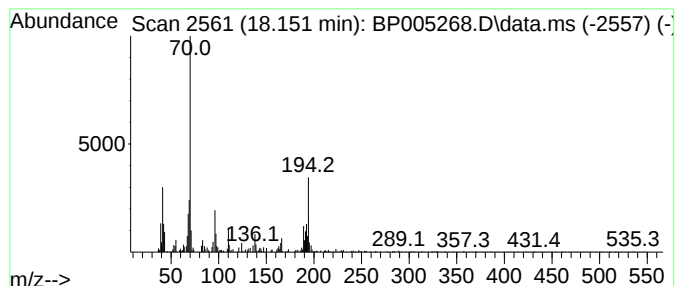
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 unknown18.15 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	2.06 ng	42032	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,10-Diethoxy-2,3,7,8-tetrahydro...	250	C14H22N2O2	1000190-75-5	42		
2	L-Proline, N-(3-cyclopentylpropi...	337	C20H35NO3	1000346-41-3	38		
3	Pyrrolidine, 2-(hydroxymethyl)-	101	C5H11NO	1000163-39-1	32		
4	2-Acetylpyrrolidine	113	C6H11NO	060026-20-2	32		
5	Pentadecanoic acid, 3-methylbuty...	242	C15H30O2	002306-91-4	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005268.D
Acq On : 12 Apr 2021 16:17
Operator : CG/JU
Sample : M1967-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

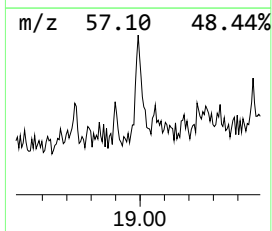
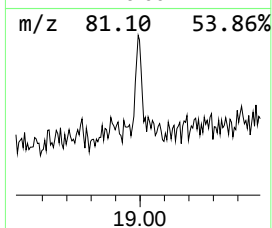
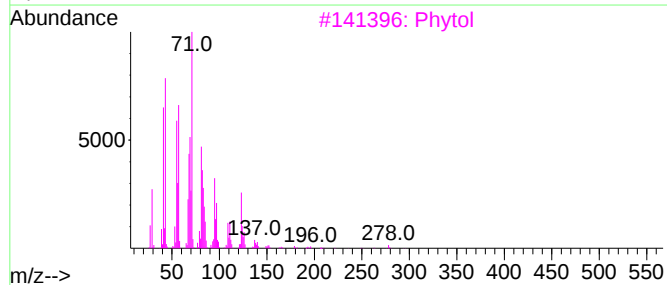
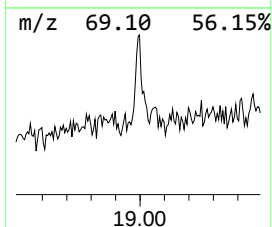
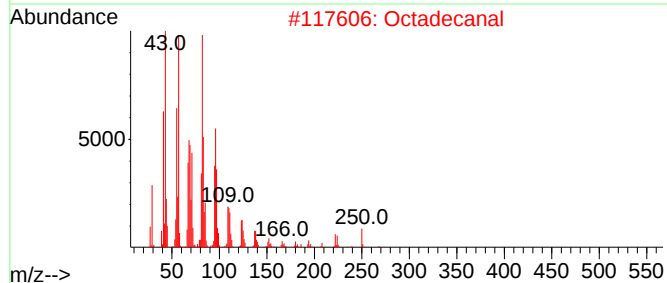
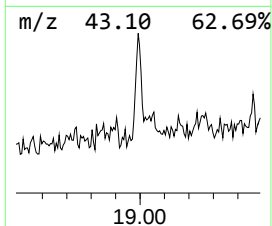
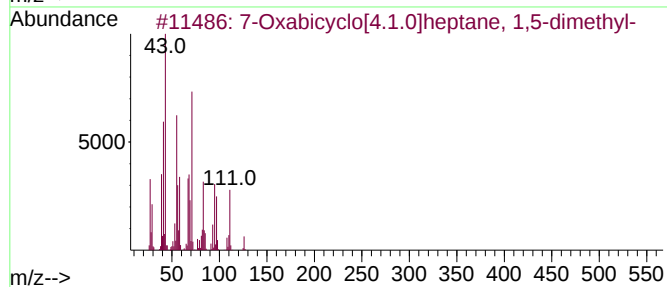
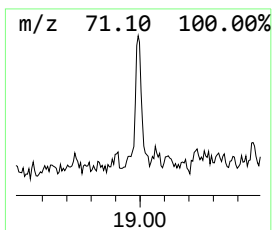
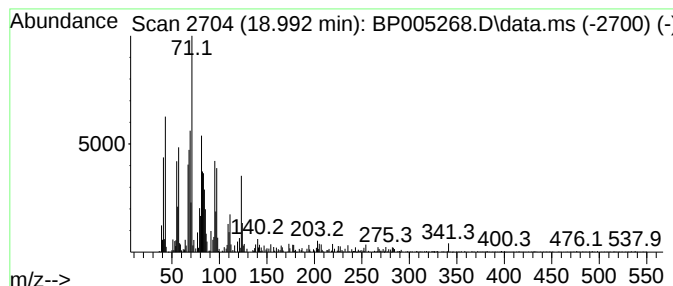
Instrument :
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ClientSampleId :
SB1-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 7-Oxabicyclo[4.1.0]heptane,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.992	3.83 ng	78148	Phenanthrene-d10		17.104	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7-Oxabicyclo[4.1.0]heptane, 1,5-...		126	C8H14O	162239-52-3	64
2	Octadecanal		268	C18H36O	000638-66-4	64
3	Phytol		296	C20H40O	000150-86-7	60
4	Levomenthol		156	C10H20O	002216-51-5	27
5	Cyclohexane, 1-methyl-4-(1-methy...		138	C10H18	001124-25-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005268.D
Acq On : 12 Apr 2021 16:17
Operator : CG/JU
Sample : M1967-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB1-C

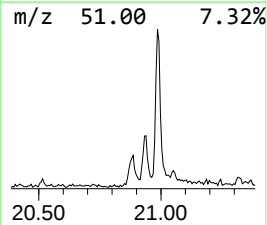
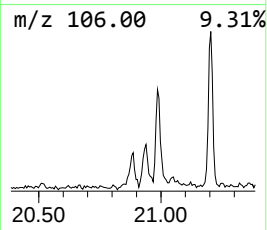
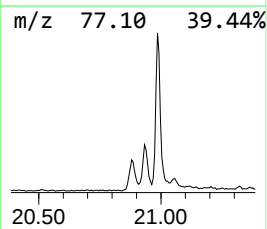
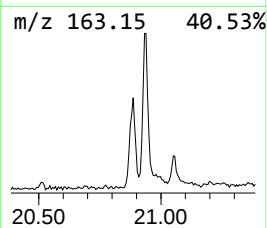
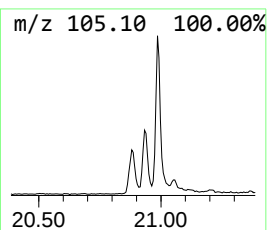
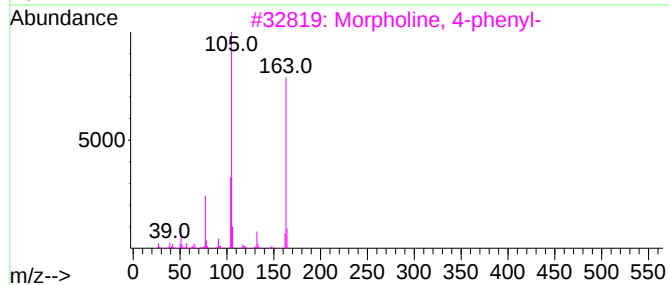
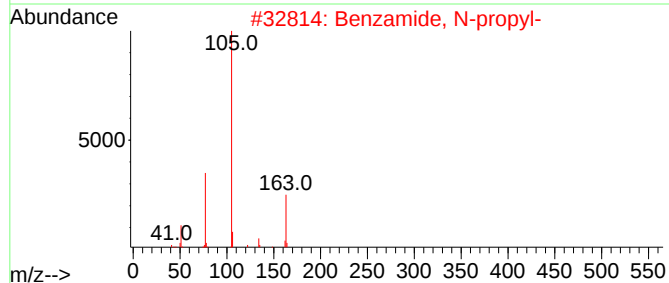
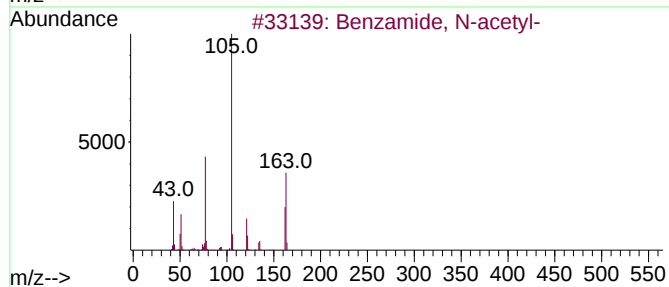
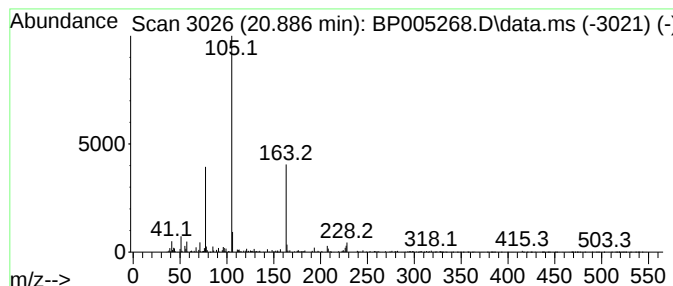
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzamide, N-acetyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	3.65 ng	98964	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	56
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	42
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	38
4			Anthraquinone, 2-benzamido-	327	C21H13NO3	052869-18-8	38
5			2-Methoxyphenyl benzoate	228	C14H12O3	000531-37-3	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005268.D
Acq On : 12 Apr 2021 16:17
Operator : CG/JU
Sample : M1967-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

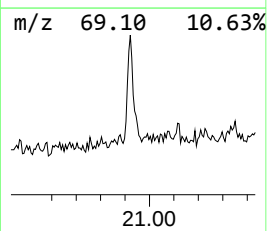
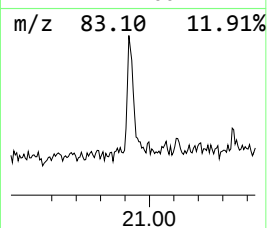
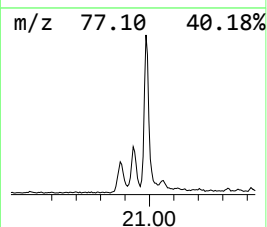
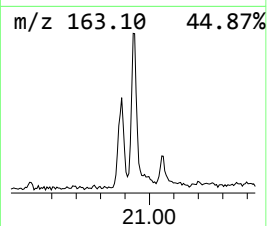
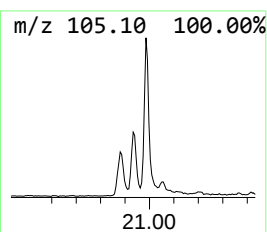
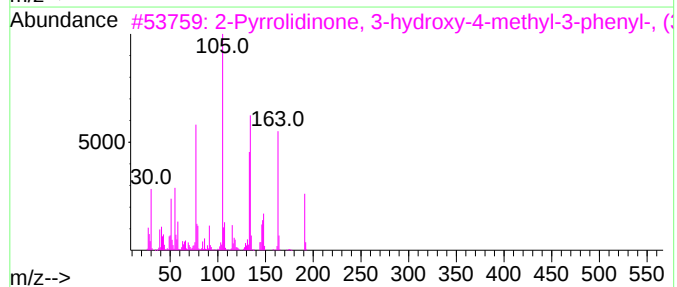
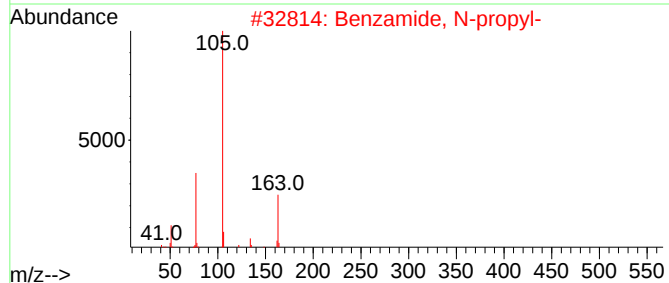
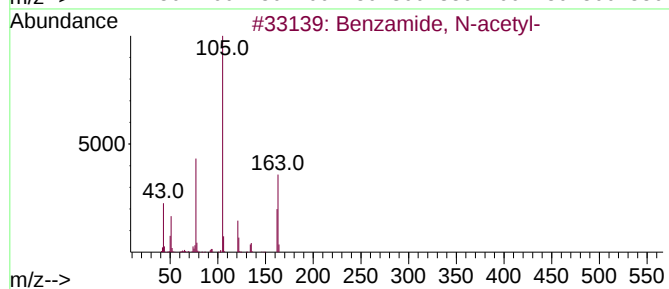
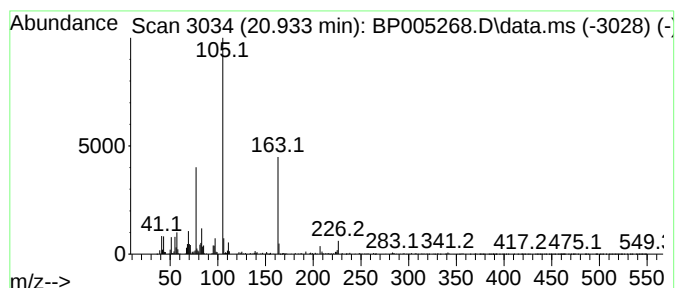
Instrument :
BNA_P
ClientSampleId :
SB1-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown20.93 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	10.98 ng	298006	Chrysene-d12	21.204
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Benzamide, N-acetyl-	163 C9H9NO2	001575-95-7 56
2		Benzamide, N-propyl-	163 C10H13NO	010546-70-0 56
3		2-Pyrrolidinone, 3-hydroxy-4-met...	191 C11H13NO2	104194-17-4 40
4		(3-Phenylloxiran-2-yl)methyl benz...	254 C16H14O3	1000366-96-1 40
5		Morpholine, 4-phenyl-	163 C10H13NO	000092-53-5 39



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005268.D
Acq On : 12 Apr 2021 16:17
Operator : CG/JU
Sample : M1967-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB1-C

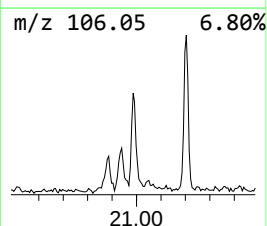
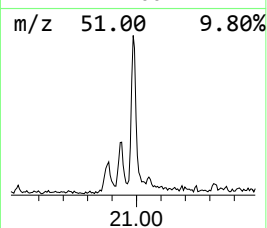
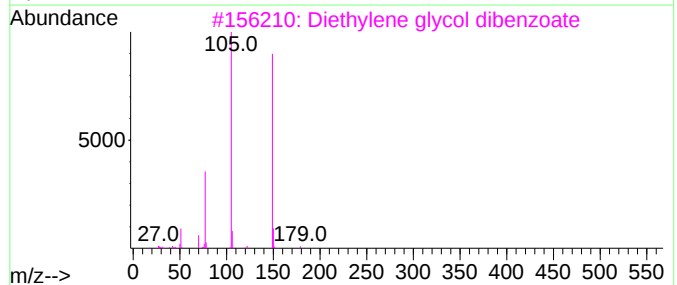
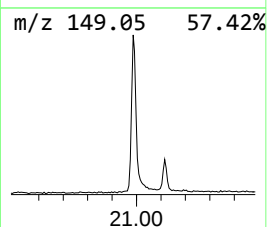
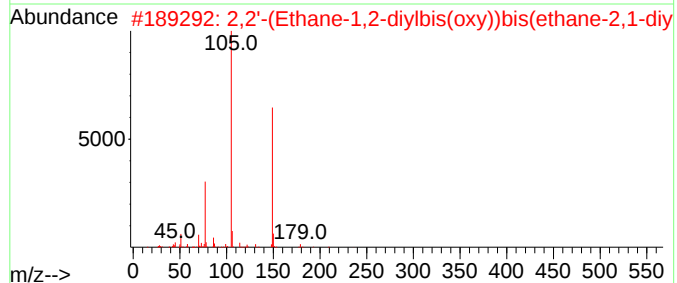
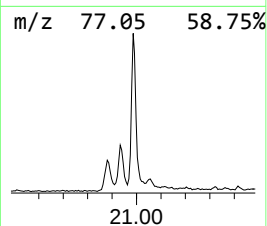
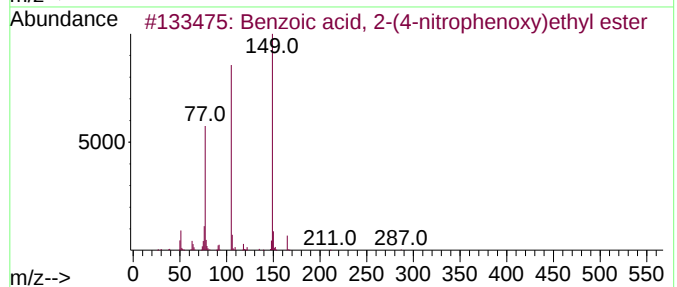
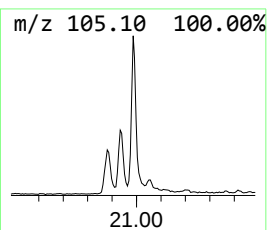
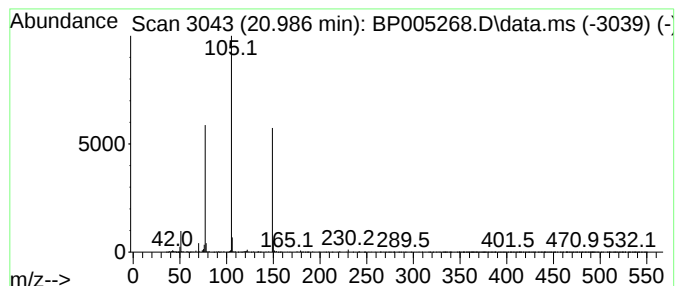
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzoic acid, 2-(4-nitrophe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	12.22 ng	331662	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	56
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	56
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
4			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	50
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005268.D
Acq On : 12 Apr 2021 16:17
Operator : CG/JU
Sample : M1967-11
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB1-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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
2-Pentanone, 4-...	4.816	37.7	ng	389568	1	7.675	206455	20.0
Indole	11.981	5.0	ng	62048	2	10.463	247643	20.0
unknown14.93	14.939	3.2	ng	51096	3	14.339	317947	20.0
2-Pentadecanone...	17.198	2.2	ng	45184	4	17.104	407658	20.0
unknown18.15	18.151	2.1	ng	42032	4	17.104	407658	20.0
7-Oxabicyclo[4....	18.992	3.8	ng	78148	4	17.104	407658	20.0
Benzamide, N-ac...	20.886	3.6	ng	98964	5	21.204	542961	20.0
unknown20.93	20.933	11.0	ng	298006	5	21.204	542961	20.0
Benzoic acid, 2...	20.986	12.2	ng	331662	5	21.204	542961	20.0