

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
 Data File : BF132700.D
 Acq On : 08 Mar 2023 20:32
 Operator : CG\JU
 Sample : 01829-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-07-20230306

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_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132700.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.216	443	447	457	rVB	1207428	1407002	46.96%	6.016%
2	5.616	510	515	526	rBV	2781949	2729163	91.08%	11.670%
3	6.610	680	684	696	rBV	2710083	2703339	90.22%	11.559%
4	6.987	745	748	752	rBV	1105147	841487	28.08%	3.598%
5	7.551	840	844	847	rBV	2067565	1726584	57.62%	7.383%
6	8.269	963	966	970	rBV	1233833	1040968	34.74%	4.451%
7	9.345	1145	1149	1152	rBV	3729616	2996337	100.00%	12.812%
8	10.033	1262	1266	1269	rVB	1283644	1089105	36.35%	4.657%
9	10.745	1383	1387	1393	rBV	147920	124594	4.16%	0.533%
10	10.822	1396	1400	1404	rBV	1708066	1541863	51.46%	6.593%
11	11.292	1477	1480	1483	rVB	71402	54075	1.80%	0.231%
12	11.374	1490	1494	1497	rBV	168246	131806	4.40%	0.564%
13	11.527	1516	1520	1524	rBV	1137051	981676	32.76%	4.198%
14	12.039	1603	1607	1611	rBV	250401	241537	8.06%	1.033%
15	12.074	1611	1613	1624	rVB	48604	60150	2.01%	0.257%
16	12.221	1633	1638	1640	rBV2	32770	47960	1.60%	0.205%
17	12.286	1646	1649	1653	rBV	70023	63054	2.10%	0.270%
18	12.827	1738	1741	1746	rBV2	60200	72957	2.43%	0.312%
19	13.116	1786	1790	1793	rBV	2805216	2374659	79.25%	10.154%
20	13.974	1933	1936	1939	rBV	159059	155181	5.18%	0.664%
21	14.004	1939	1941	1952	rVB	163311	246296	8.22%	1.053%
22	14.145	1962	1965	1968	rBV	73007	64964	2.17%	0.278%
23	14.186	1968	1972	1979	rVB	1029552	931048	31.07%	3.981%
24	14.310	1990	1993	1997	rBV	225697	191133	6.38%	0.817%
25	14.351	1997	2000	2002	rVV	310867	266246	8.89%	1.138%
26	14.380	2002	2005	2007	rVV	99127	96812	3.23%	0.414%
27	14.398	2007	2008	2011	rVB	101908	80360	2.68%	0.344%
28	14.633	2045	2048	2055	rBV5	20658	35837	1.20%	0.153%
29	14.698	2057	2059	2062	rVV	42639	40072	1.34%	0.171%
30	15.727	2229	2234	2241	rBV	768074	1050290	35.05%	4.491%

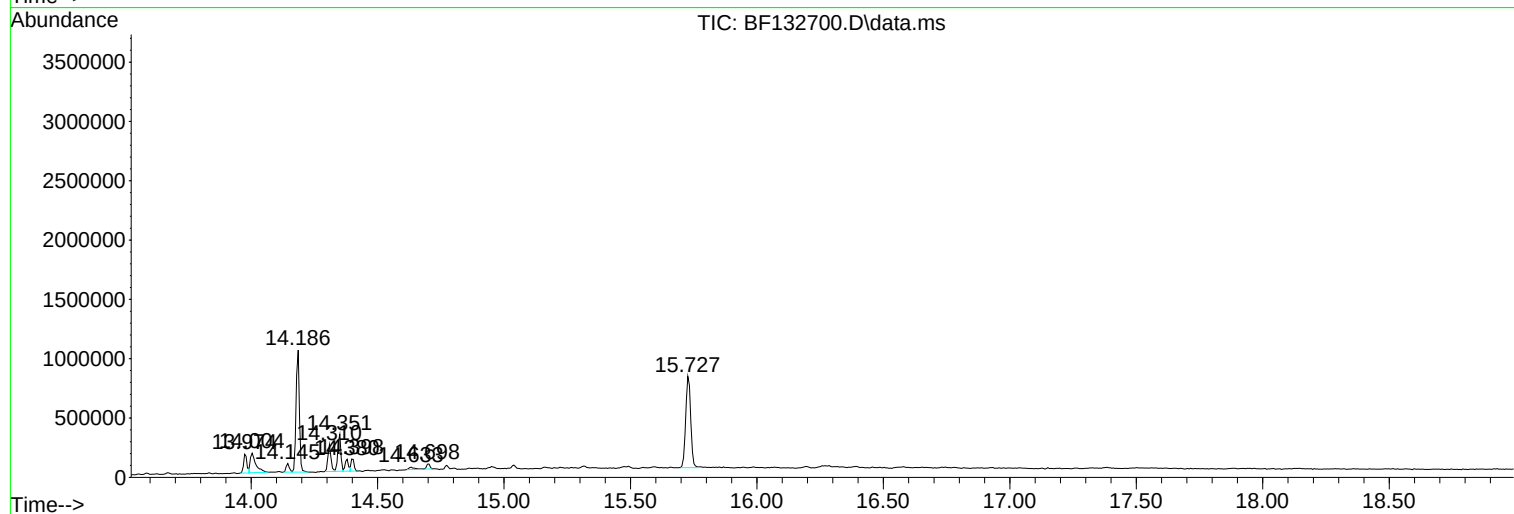
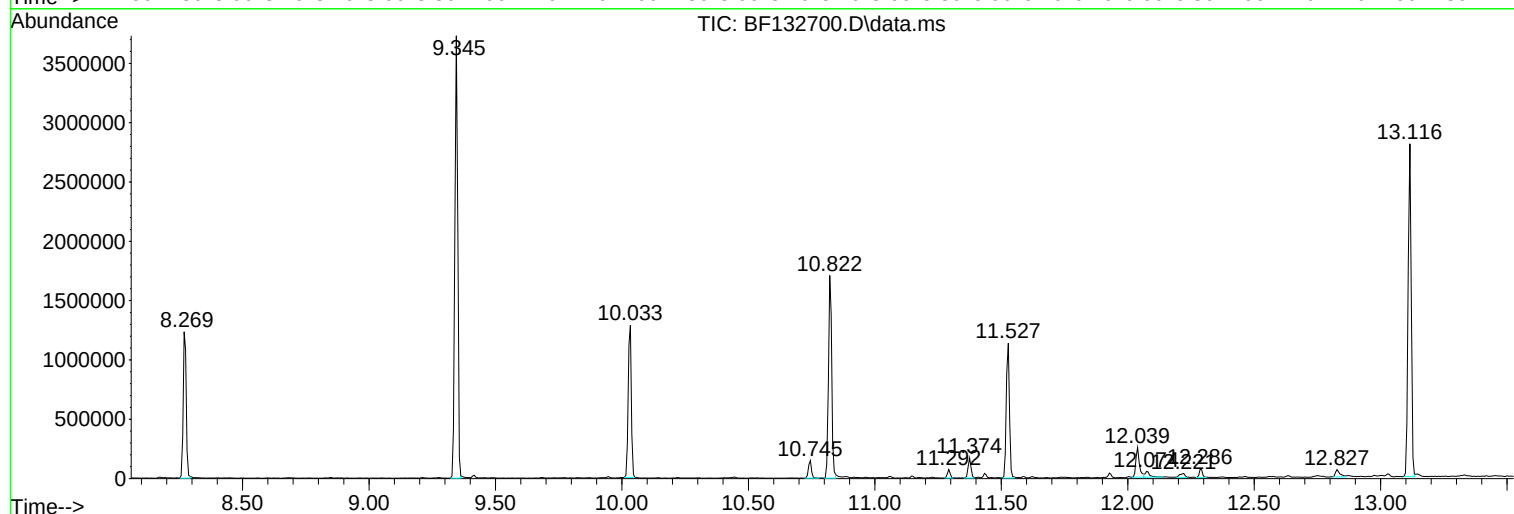
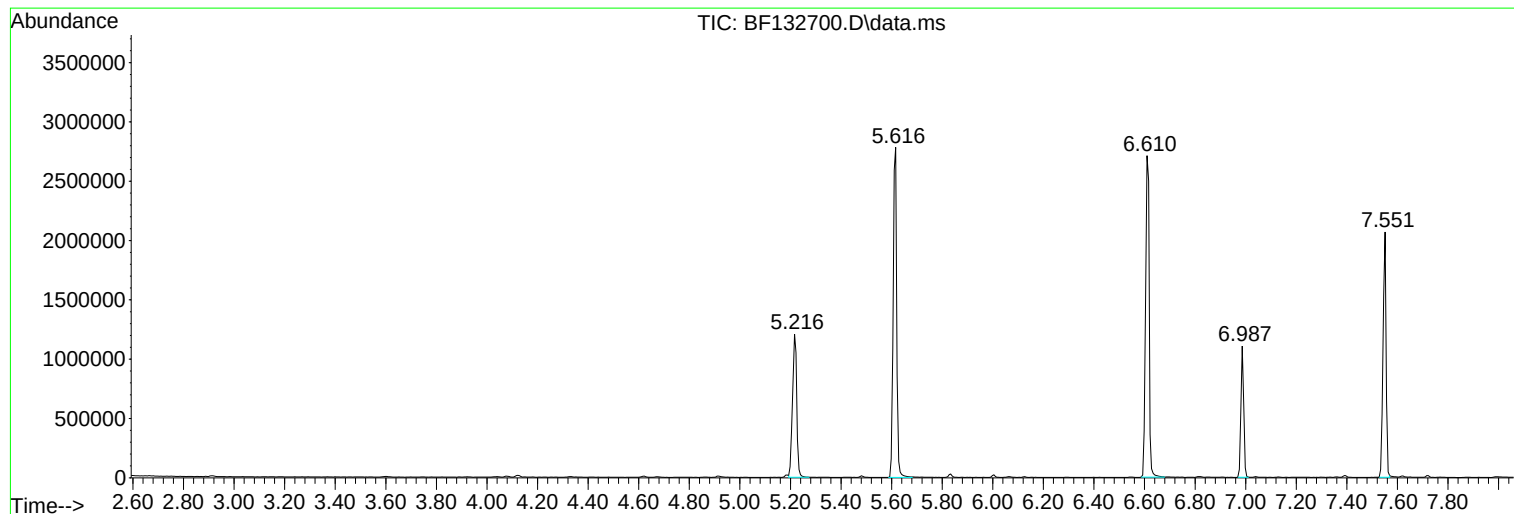
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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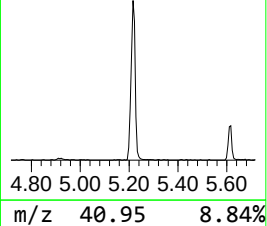
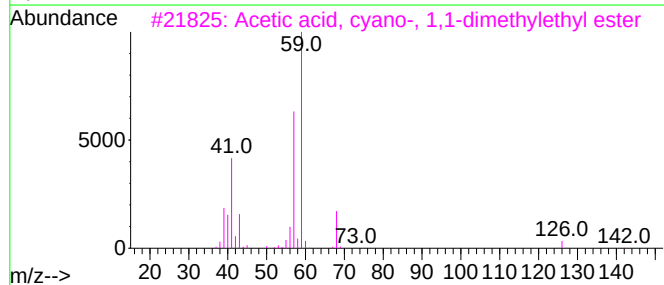
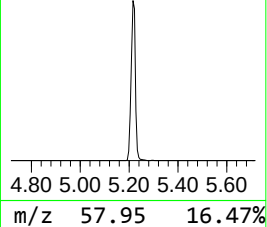
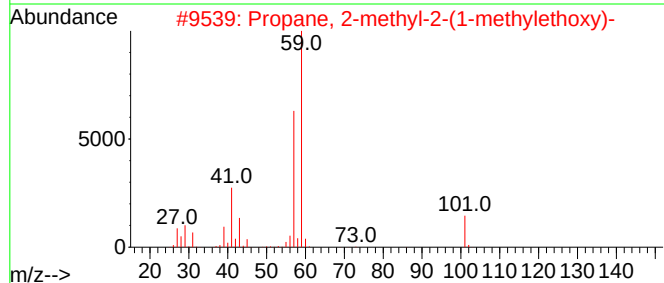
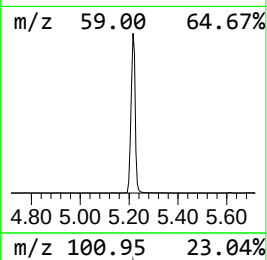
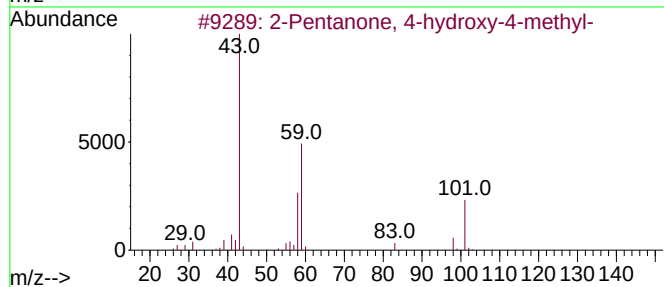
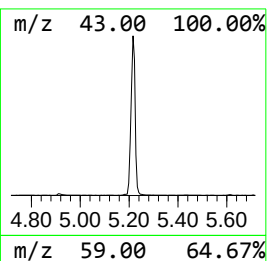
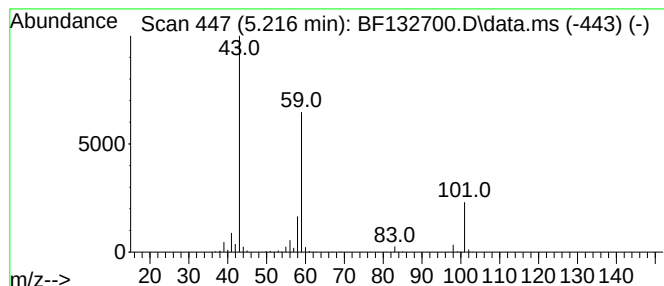
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.216	33.44 ng	1407000	1,4-Dichlorobenzene-d4	6.987

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Guanidine	59	CH5N3	000113-00-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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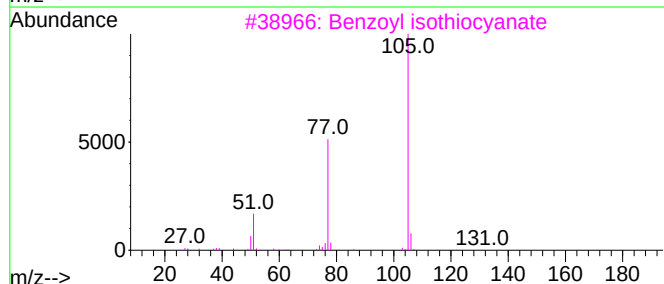
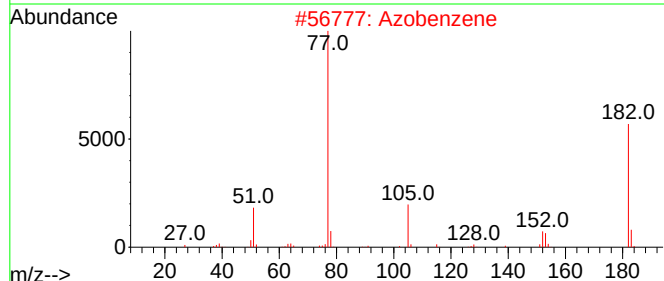
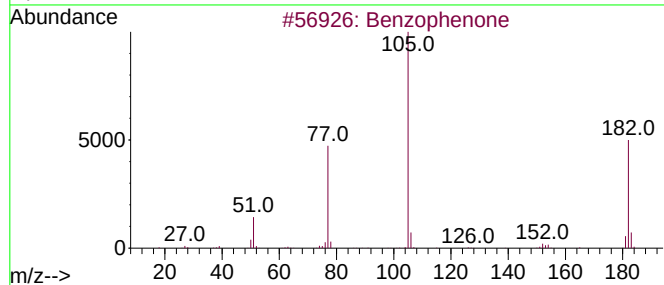
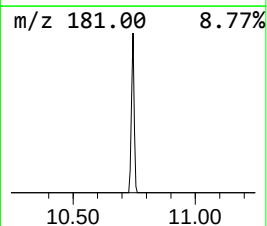
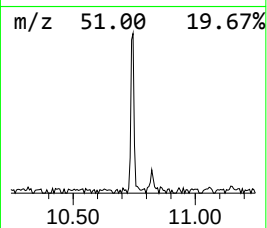
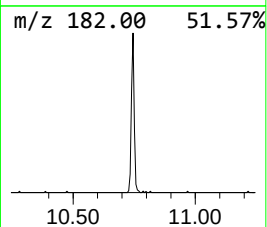
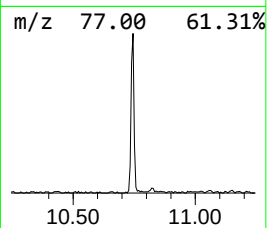
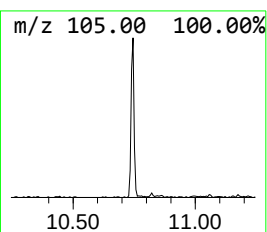
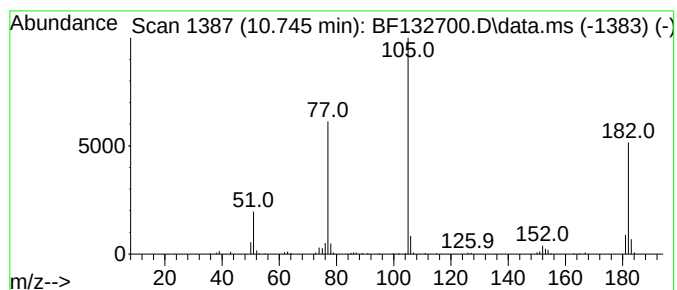
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Peak Number 2 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.745	2.29 ng	124594	Acenaphthene-d10	10.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	49
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			Phenacylidene diacetate	236	C12H12O5	005062-30-6	47



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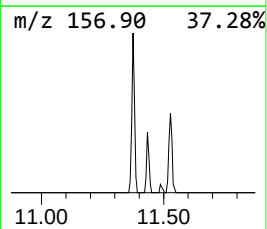
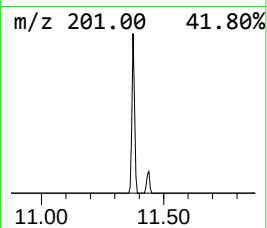
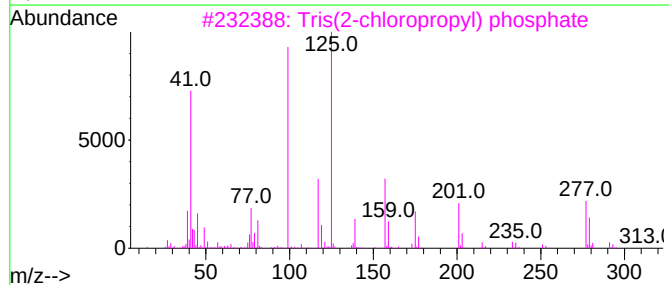
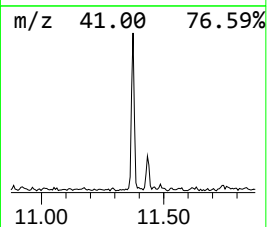
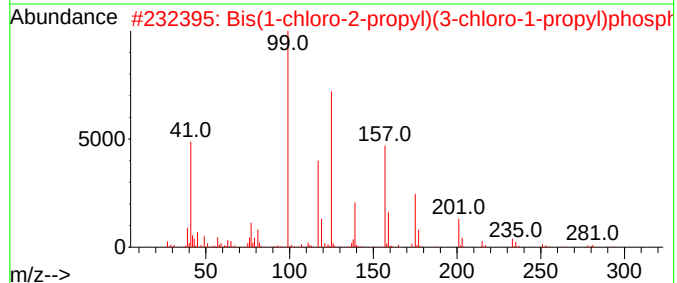
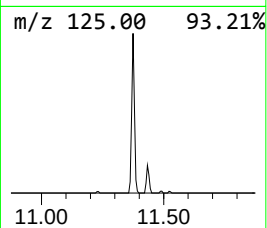
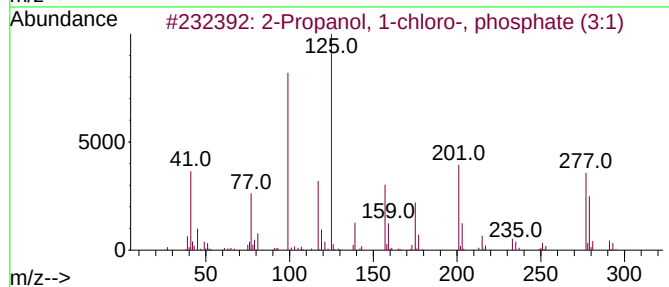
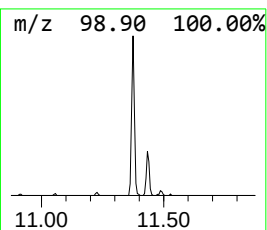
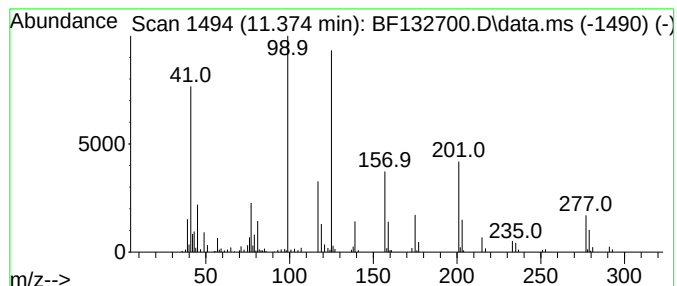
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Propanol, 1-chloro-, phos... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.374	2.69 ng	131806	Phenanthrene-d10	11.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-chloro-, phosphate...	326	C9H18Cl3O4P	013674-84-5	68
2	Bis(1-chloro-2-propyl)(3-chloro-...	326	C9H18Cl3O4P	137909-40-1	38
3	Tris(2-chloropropyl) phosphate	326	C9H18Cl3O4P	006145-73-9	38
4	Bis(3-chloro-1-propyl)(1-chloro-...	326	C9H18Cl3O4P	137888-35-8	37
5	Sarin	140	C4H10F02P	000107-44-8	25



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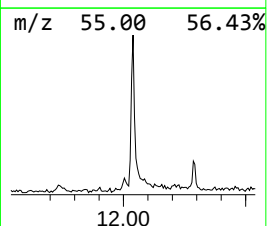
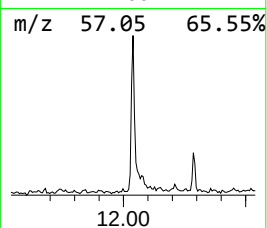
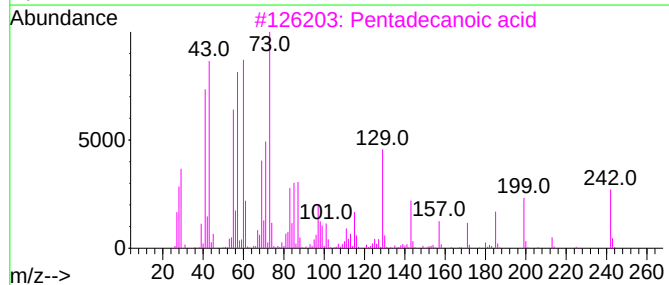
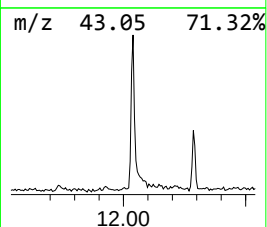
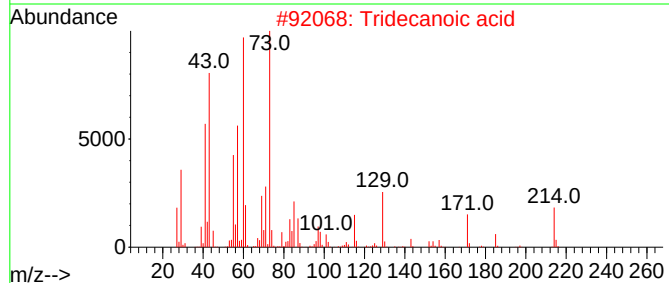
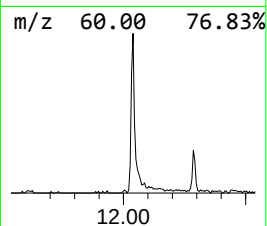
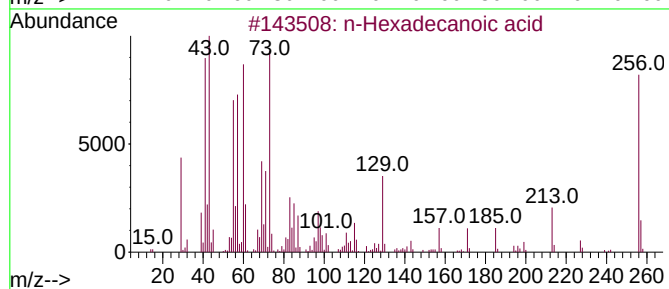
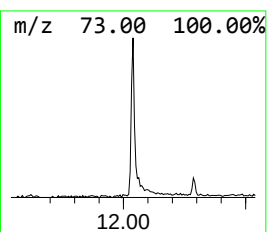
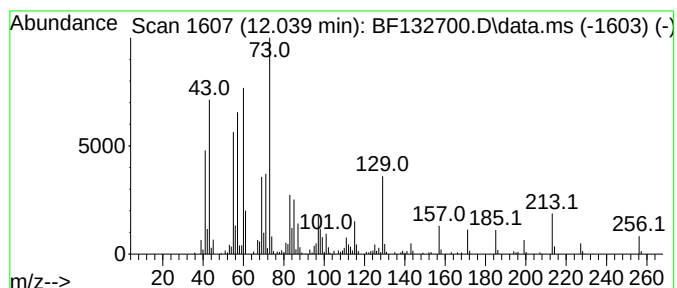
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.039	4.92 ng	241537	Phenanthrene-d10	11.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			Trehalose	342	C12H22O11	000099-20-7	50



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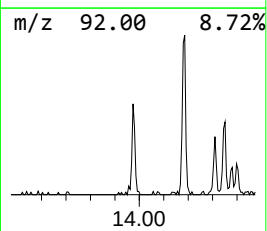
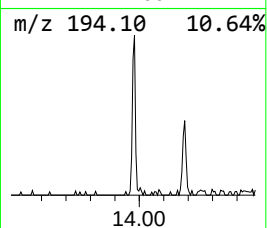
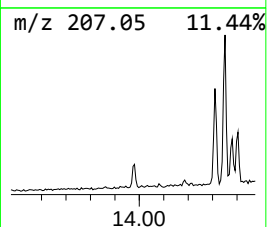
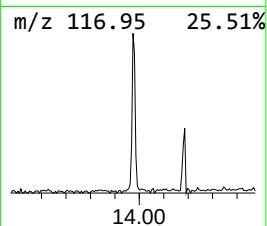
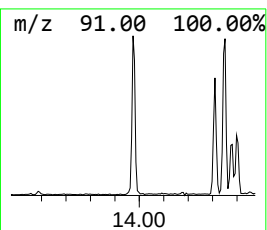
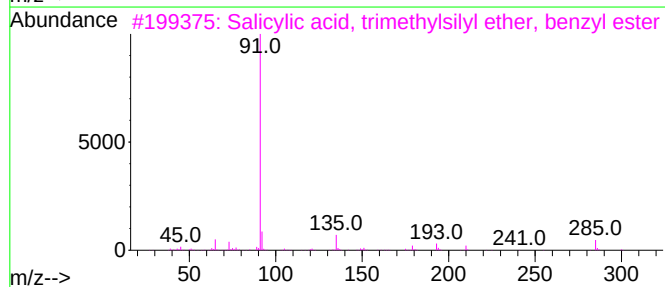
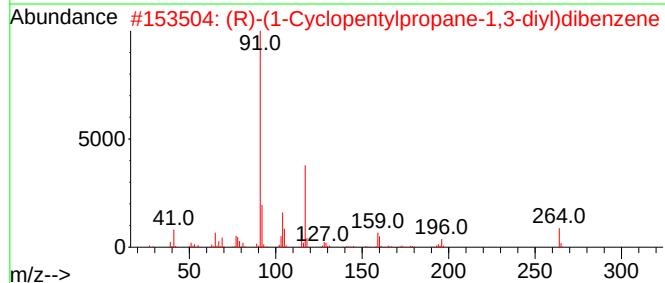
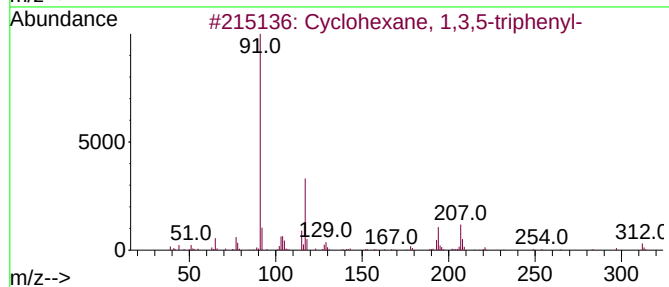
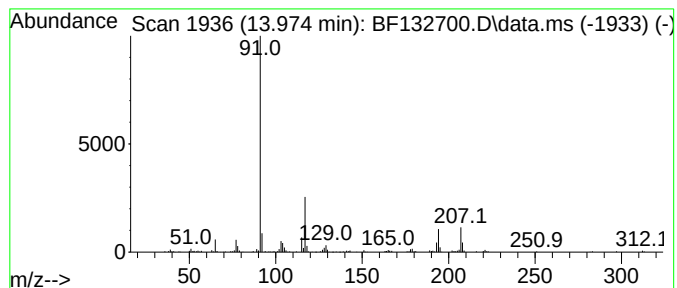
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Peak Number 5 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	3.33 ng	155181	Chrysene-d12	14.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	90
2			(R)-(1-Cyclopentylpropane-1,3-di...	264	C20H24	1402851-74-4	32
3			Salicylic acid, trimethylsilyl e...	300	C17H20O3Si	1000463-82-7	22
4			Carbonic acid, monoamide, N-benz...	207	C12H17NO2	1000451-48-5	16
5			Nialamide, 1TMS derivative	370	C19H26N4O2Si	1000485-79-3	16



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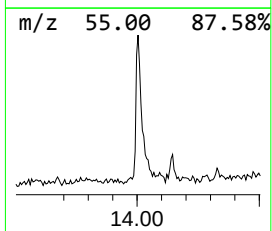
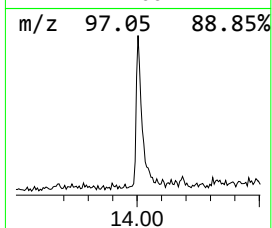
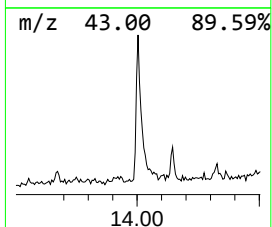
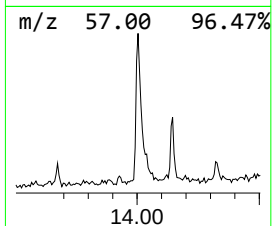
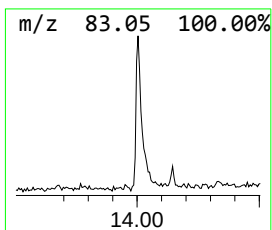
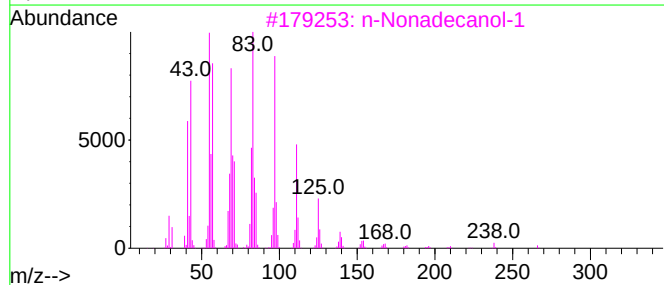
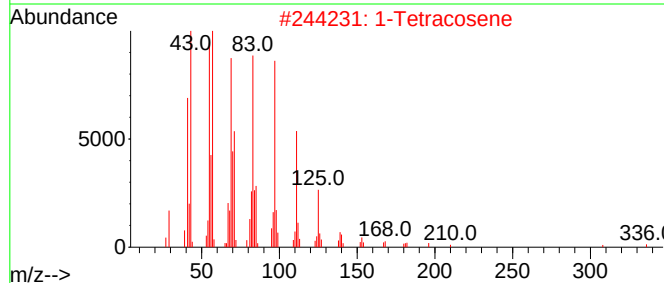
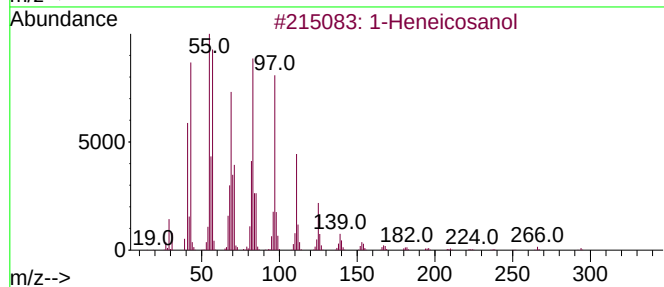
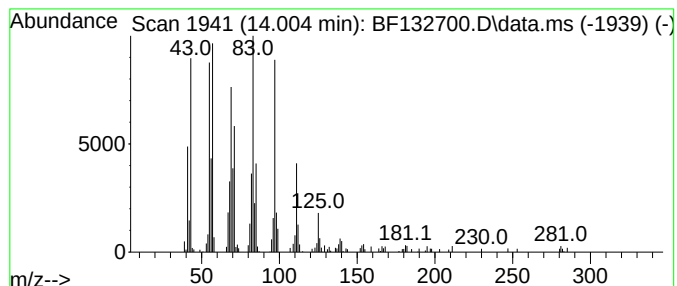
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	5.29 ng	246296	Chrysene-d12	14.186

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		1-Tetracosene	336	C24H48	010192-32-2	91
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5		Behenic alcohol	326	C22H46O	000661-19-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132700.D
Acq On : 08 Mar 2023 20:32
Operator : CG\JU
Sample : 01829-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-07-20230306

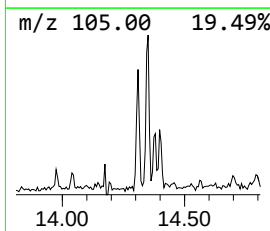
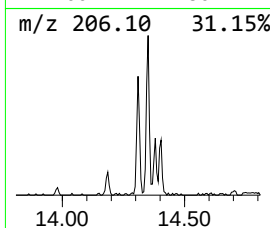
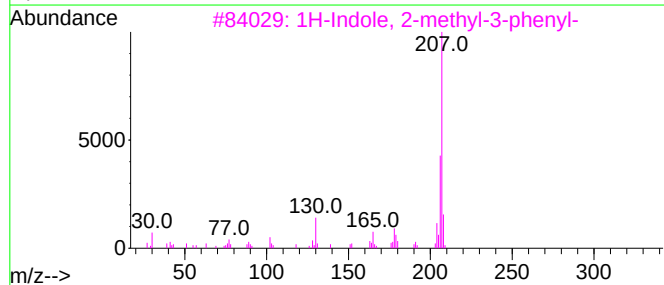
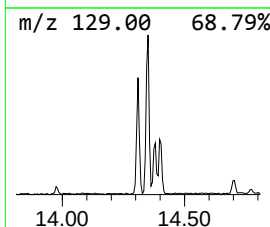
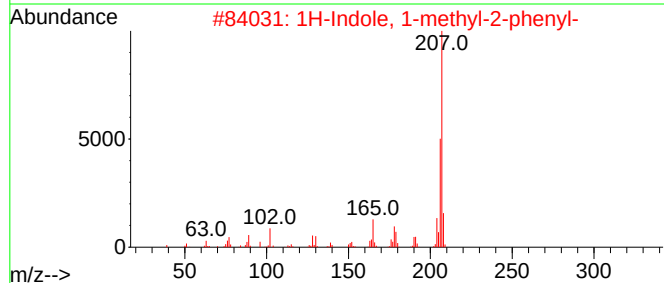
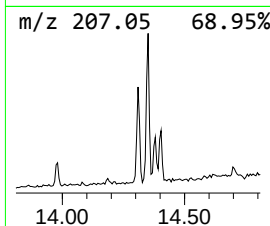
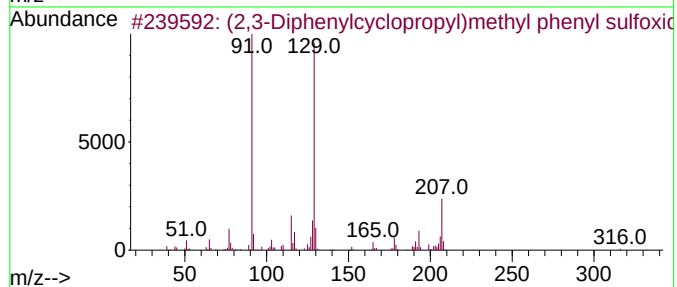
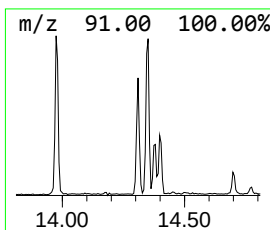
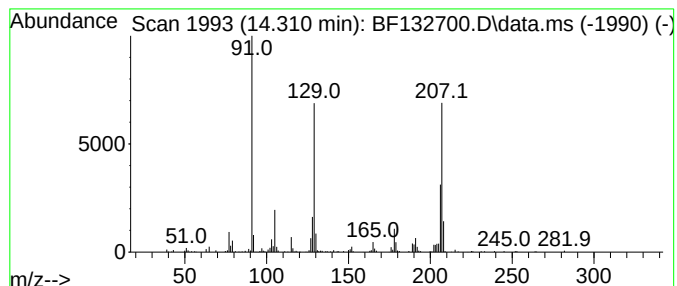
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.310 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.310	4.11 ng	191133	Chrysene-d12	14.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	43
2			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	41
3			1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	38
4			7-Methyl -2-phenyl-1H-indole	207	C15H13N	059541-82-1	38
5			5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132700.D
Acq On : 08 Mar 2023 20:32
Operator : CG\JU
Sample : 01829-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-07-20230306

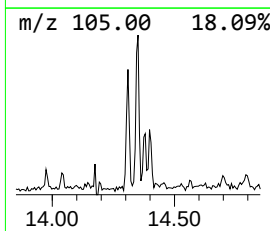
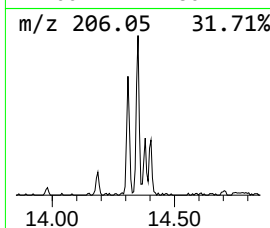
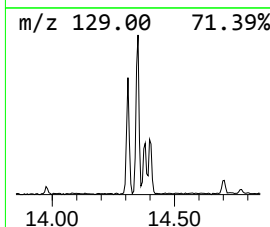
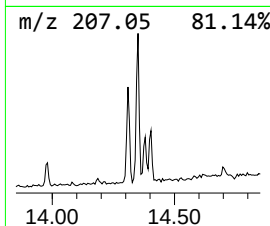
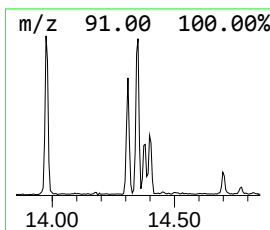
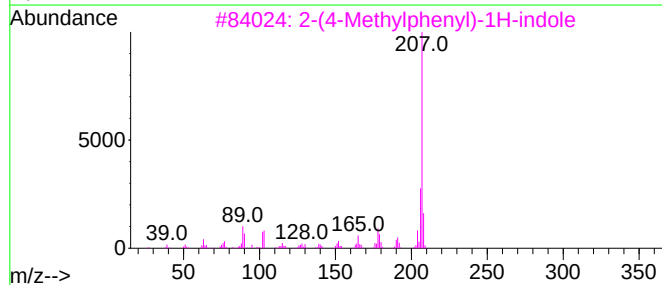
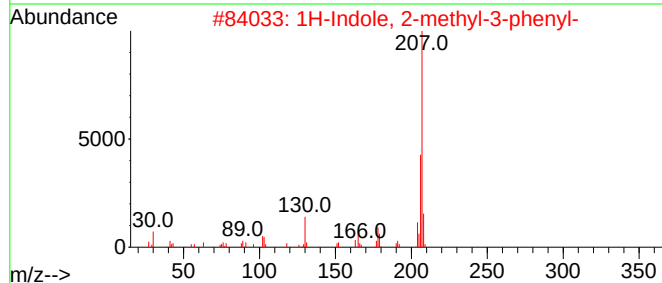
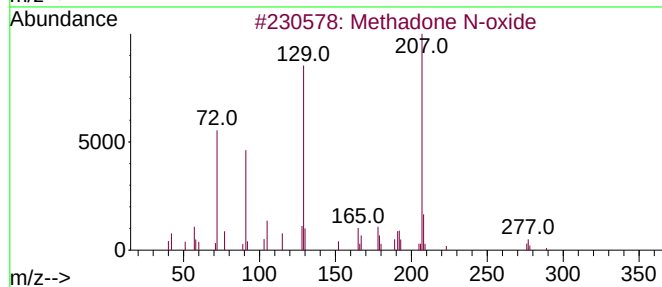
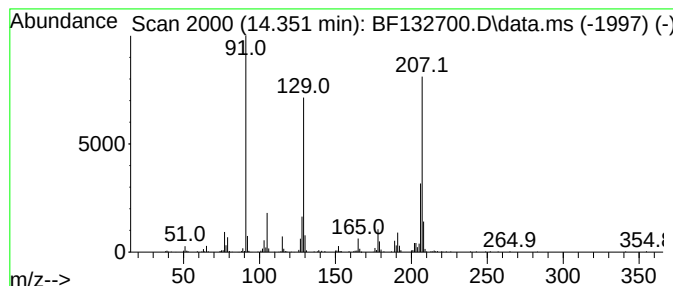
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methadone N-oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	5.72 ng	266246	Chrysene-d12	14.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
2			1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	60
3			2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	55
4			1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	53
5			Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132700.D
Acq On : 08 Mar 2023 20:32
Operator : CG\JU
Sample : 01829-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

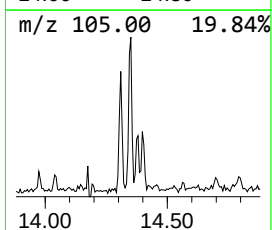
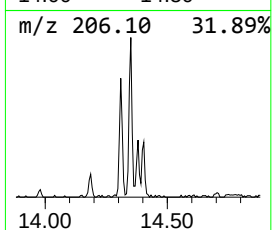
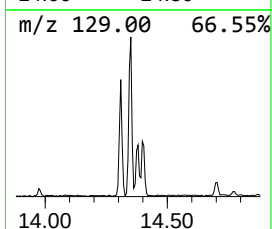
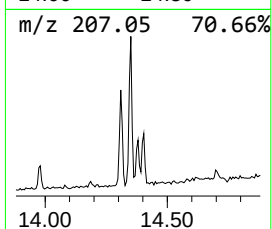
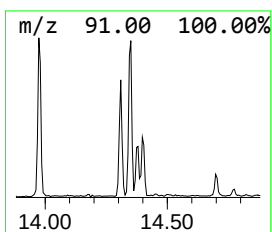
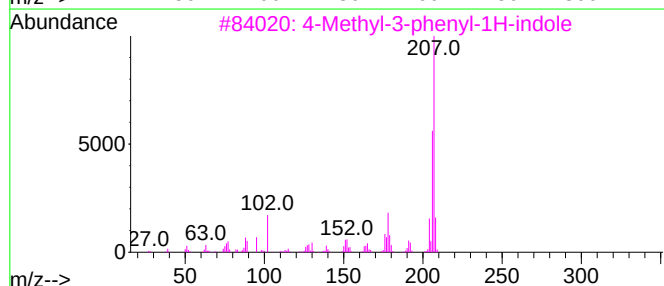
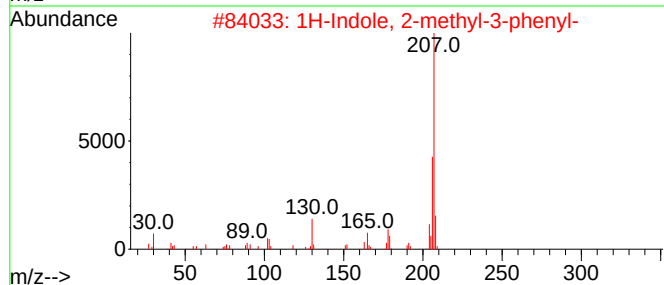
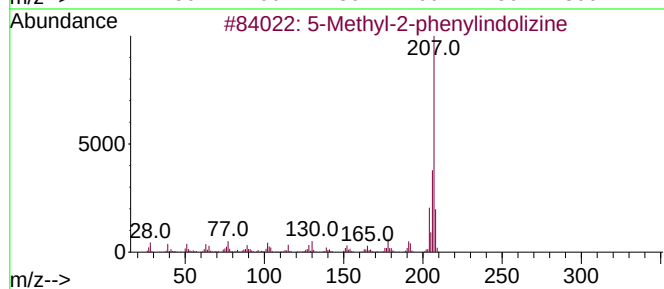
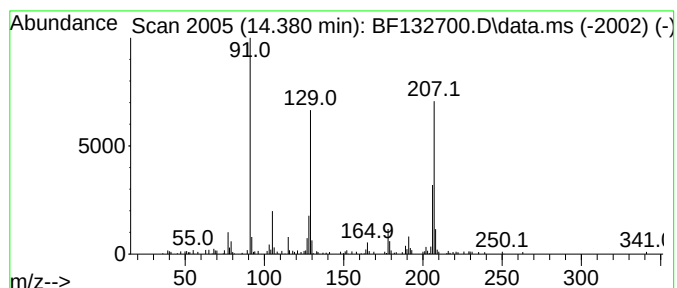
Instrument :
BNA_F
ClientSampleId :
SS-07-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.380 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.380	2.08 ng	96812	Chrysene-d12	14.186	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	41
2	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	41
3	4-Methyl-3-phenyl-1H-indole	207	C15H13N	180271-54-9	38
4	7-Methyl -2-phenyl-1H-indole	207	C15H13N	059541-82-1	38
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132700.D
Acq On : 08 Mar 2023 20:32
Operator : CG\JU
Sample : 01829-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-07-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.216	33.4	ng	1407000	1	6.987	841487	20.0
Benzophenone	10.745	2.3	ng	124594	3	10.033	1089110	20.0
2-Propanol, 1-c...	11.374	2.7	ng	131806	4	11.527	981676	20.0
n-Hexadecanoic ...	12.039	4.9	ng	241537	4	11.527	981676	20.0
Cyclohexane, 1,...	13.974	3.3	ng	155181	5	14.186	931048	20.0
1-Heneicosanol	14.004	5.3	ng	246296	5	14.186	931048	20.0
unknown14.310	14.310	4.1	ng	191133	5	14.186	931048	20.0
Methadone N-oxide	14.351	5.7	ng	266246	5	14.186	931048	20.0
unknown14.380	14.380	2.1	ng	96812	5	14.186	931048	20.0