

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
 Data File : BF134650.D
 Acq On : 07 Aug 2023 12:58
 Operator : CG\JU
 Sample : 03887-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MCLEAN-TP6

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134650.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.893	303	307	312	rVB	103160	131351	3.38%	0.425%
2	5.040	498	502	510	rVB	55493	67298	1.73%	0.218%
3	5.434	563	569	572	rBV	3665731	3699922	95.16%	11.964%
4	6.434	733	739	742	rBV	3675764	3676407	94.56%	11.888%
5	6.798	797	801	804	rBV	1706543	1326934	34.13%	4.291%
6	7.357	891	896	899	rBV	2451016	2337601	60.12%	7.559%
7	8.075	1014	1018	1022	rBV	2061013	1705733	43.87%	5.515%
8	9.157	1197	1202	1205	rBV	4282542	3888009	100.00%	12.572%
9	9.833	1313	1317	1320	rBV	1970605	1706464	43.89%	5.518%
10	10.475	1422	1426	1435	rBV	391466	323058	8.31%	1.045%
11	10.545	1435	1438	1442	rVB	447936	375513	9.66%	1.214%
12	10.622	1446	1451	1454	rBV	2337525	2100868	54.03%	6.793%
13	10.675	1456	1460	1463	rBV	853622	845481	21.75%	2.734%
14	11.322	1566	1570	1572	rBV	1754860	1483100	38.15%	4.796%
15	11.339	1572	1573	1577	rVV	89640	73507	1.89%	0.238%
16	11.392	1577	1582	1585	rVB2	68961	62266	1.60%	0.201%
17	11.857	1657	1661	1665	rBV2	264797	247837	6.37%	0.801%
18	12.533	1773	1776	1780	rBV	201308	171720	4.42%	0.555%
19	12.763	1809	1815	1818	rBV	178836	178179	4.58%	0.576%
20	12.916	1837	1841	1844	rBV	3555557	3090376	79.48%	9.993%
21	13.821	1991	1995	2000	rBV2	350370	355757	9.15%	1.150%
22	13.968	2015	2020	2023	rBV	1380513	1367511	35.17%	4.422%
23	13.992	2023	2024	2027	rVB	81095	44059	1.13%	0.142%
24	14.215	2059	2062	2066	rBV	47935	53371	1.37%	0.173%
25	14.427	2095	2098	2100	rBV	150400	136991	3.52%	0.443%
26	15.004	2193	2196	2199	rBV	75891	104919	2.70%	0.339%
27	15.110	2212	2214	2220	rVB3	50181	59538	1.53%	0.193%
28	15.309	2245	2248	2253	rVB	46156	55636	1.43%	0.180%
29	15.368	2256	2258	2262	rVB	56595	60573	1.56%	0.196%
30	15.439	2265	2270	2274	rBV	990196	1196522	30.77%	3.869%

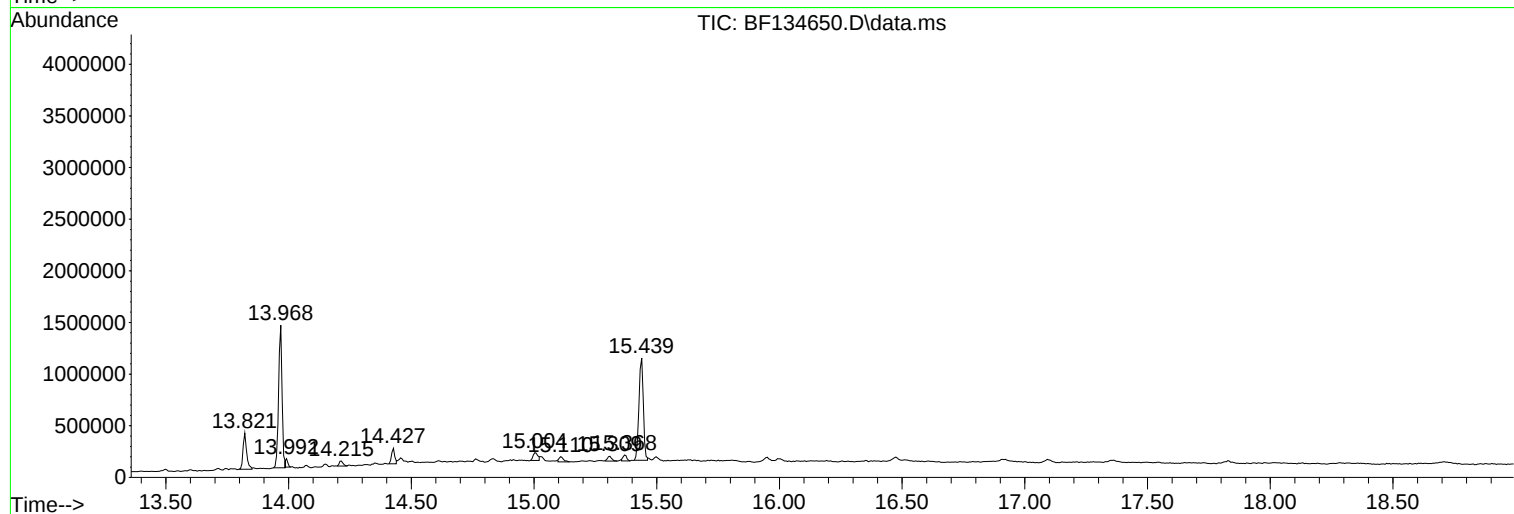
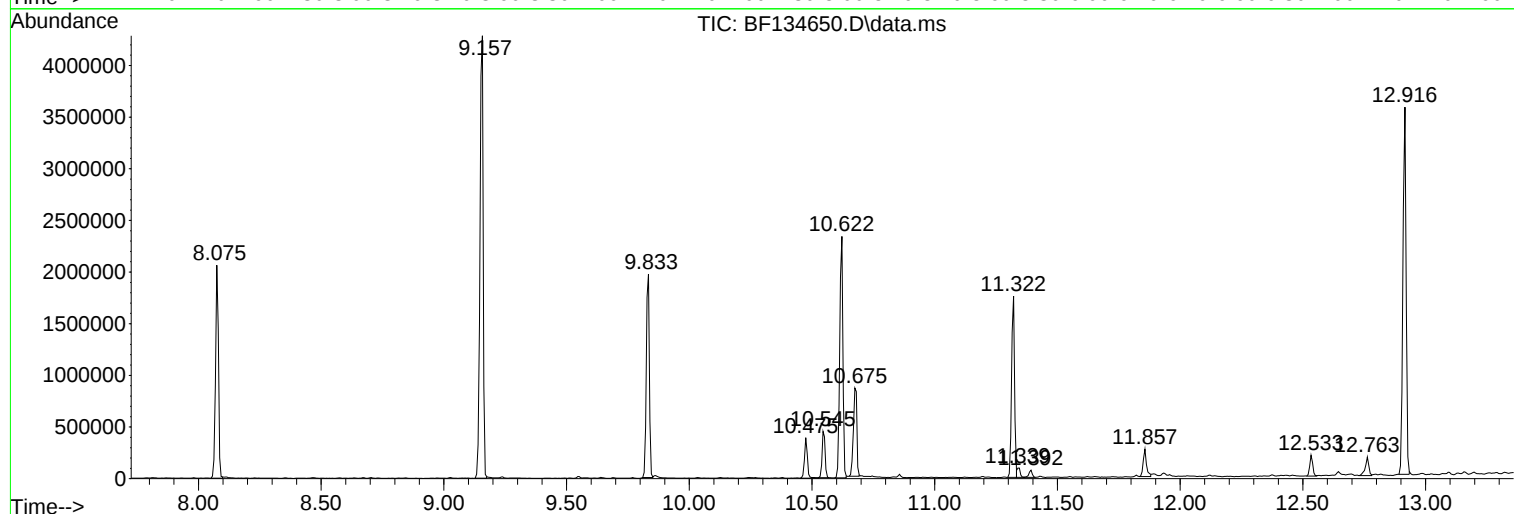
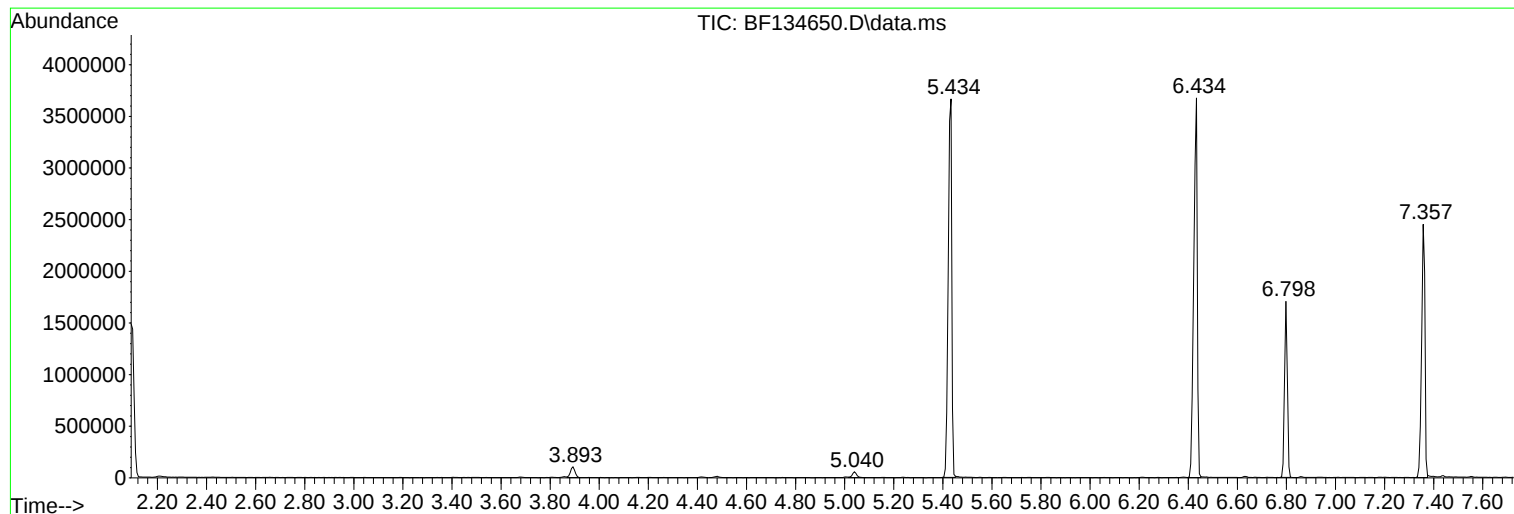
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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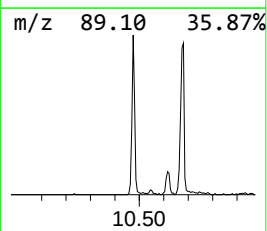
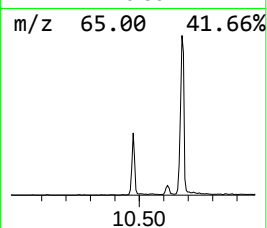
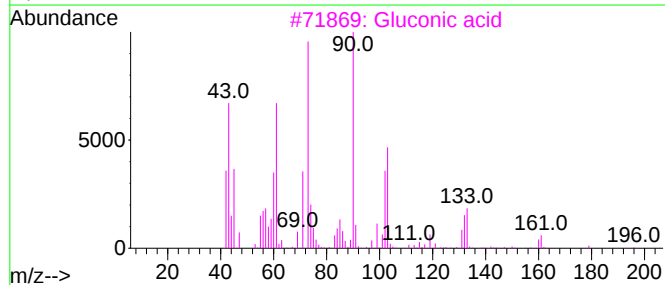
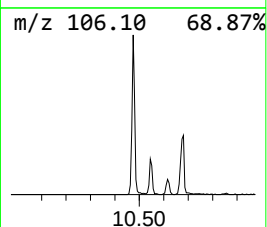
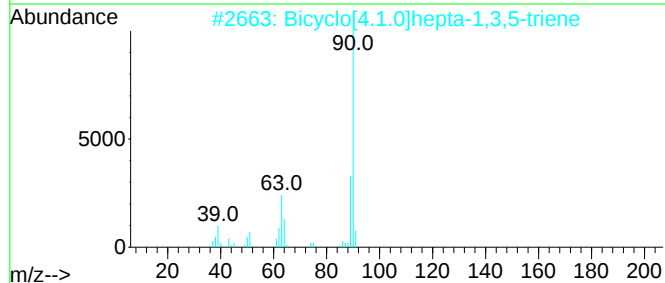
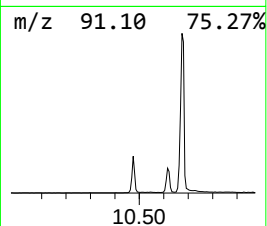
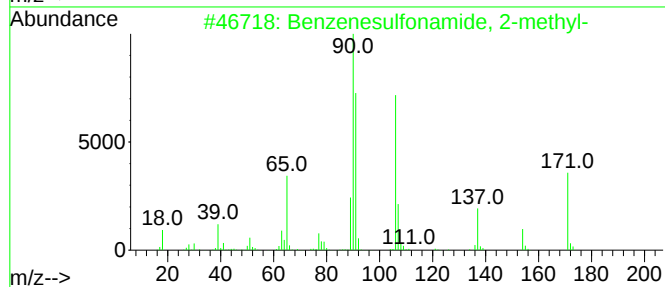
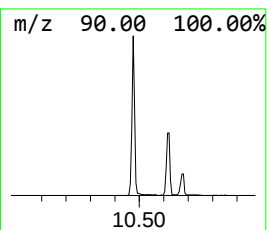
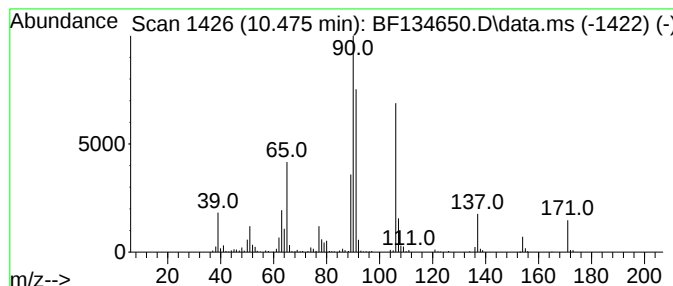
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzenesulfonamide, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.79 ng	323058	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	95
2			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	49
3			Gluconic acid	196	C6H12O7	000526-95-4	38
4			4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	28
5			Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	22



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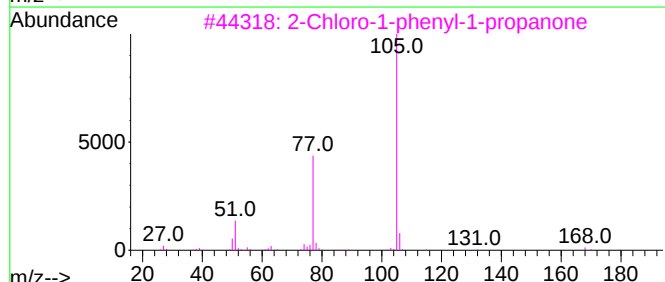
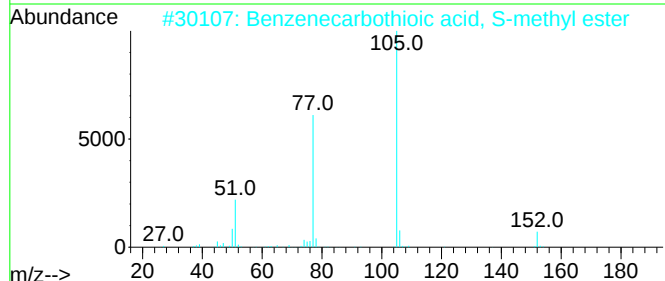
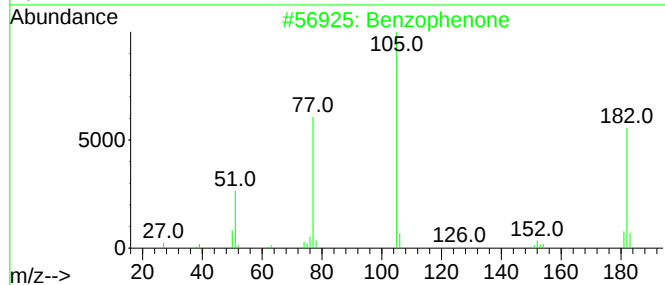
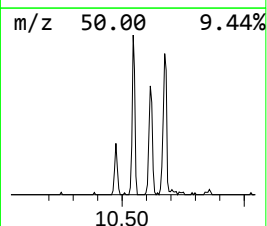
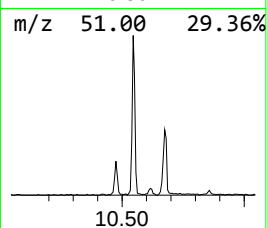
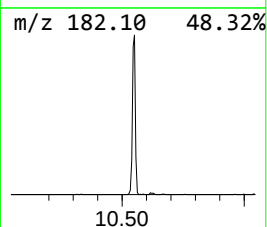
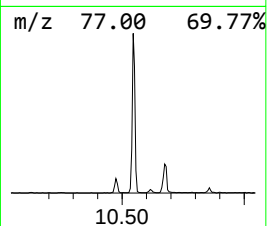
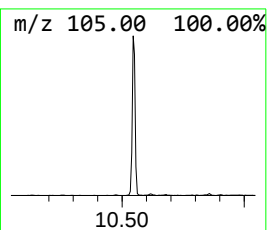
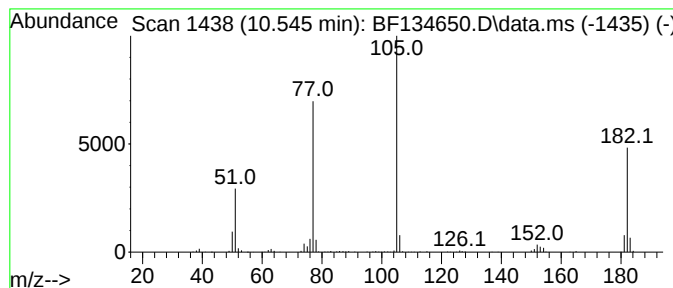
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.545	4.40 ng	375513	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	50
4			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	50
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	50



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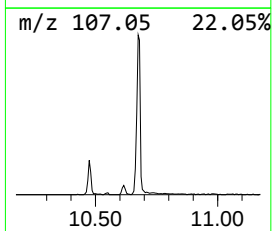
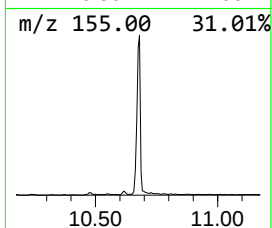
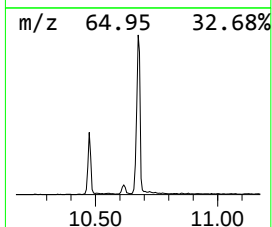
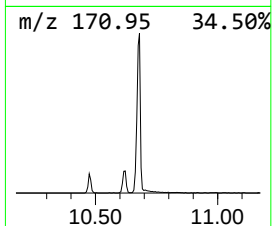
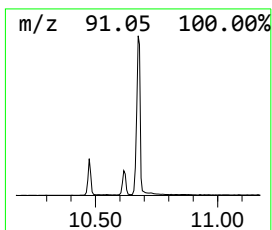
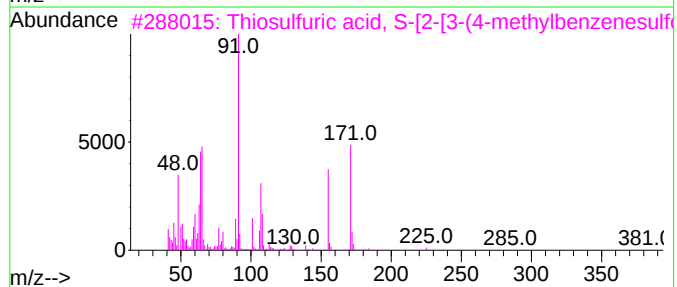
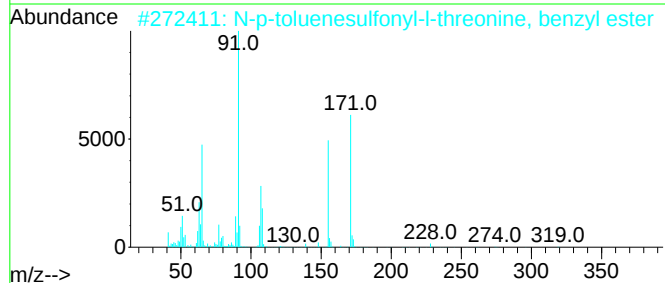
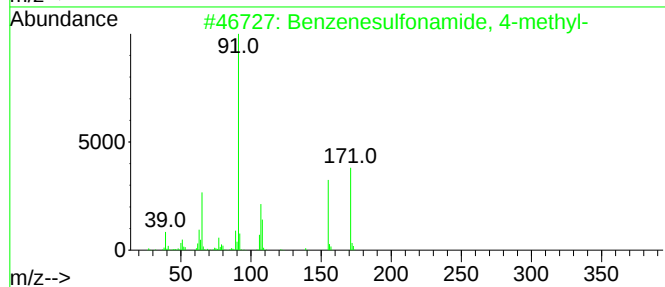
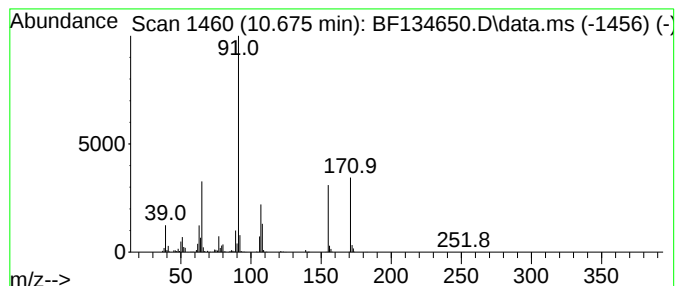
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzenesulfonamide, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.675	11.40 ng	845481	Phenanthrene-d10	11.322	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	87
3	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	83
4	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	72
5	Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	43



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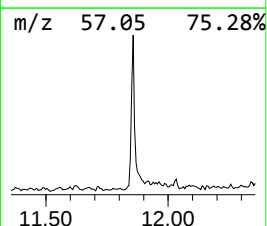
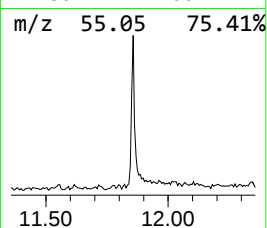
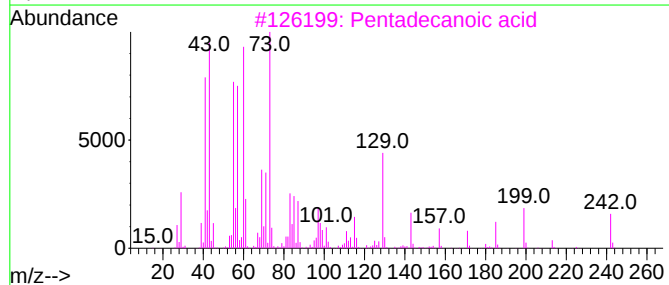
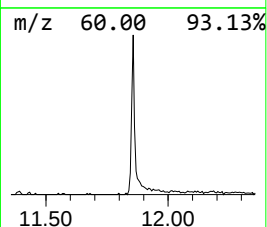
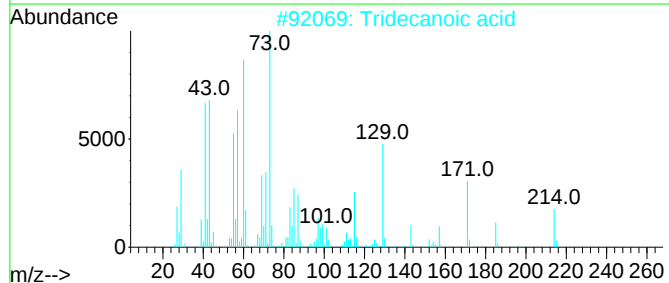
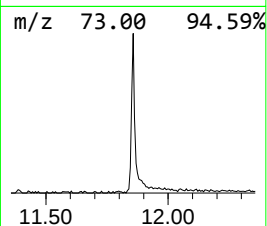
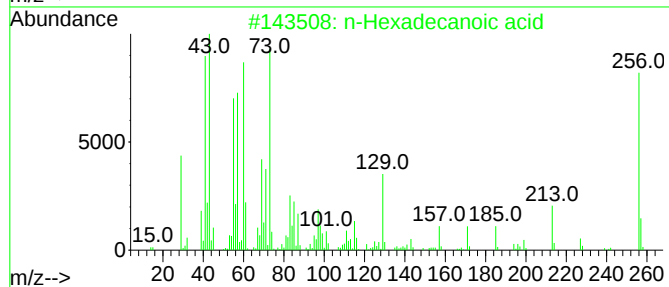
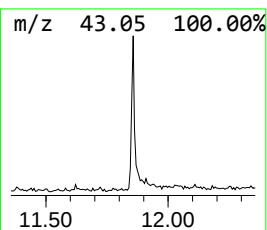
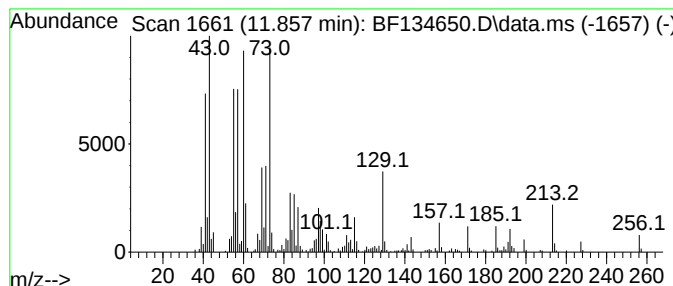
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.34 ng	247837	Phenanthrene-d10	11.322

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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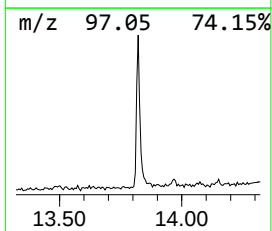
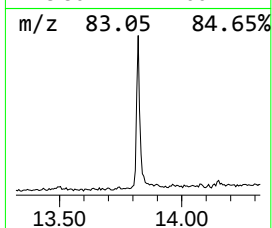
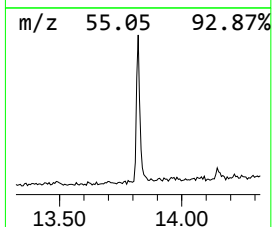
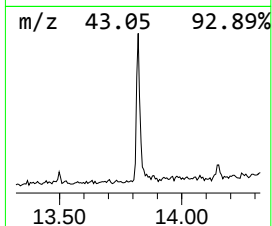
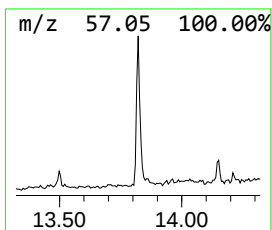
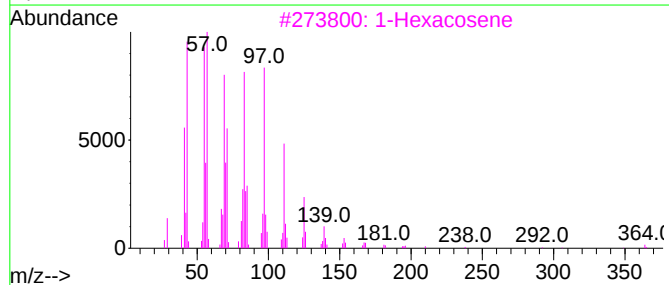
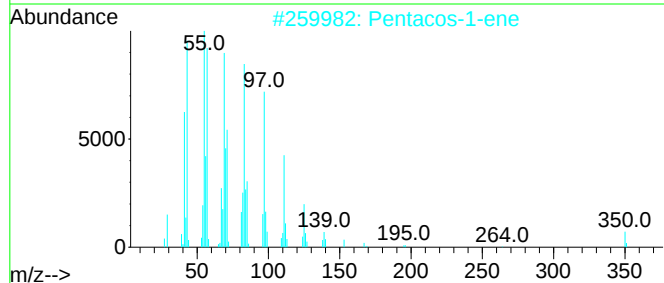
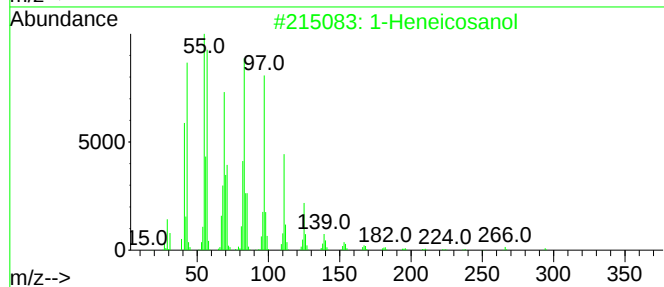
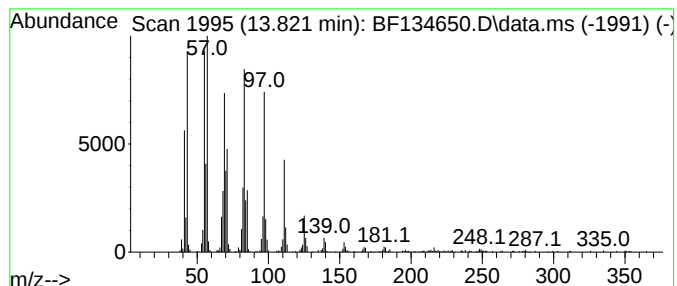
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Peak Number 6 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	5.20 ng	355757	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Pentacos-1-ene	350	C25H50	016980-85-1	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5			1-Tetracosene	336	C24H48	010192-32-2	94



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MCLEAN-TP6

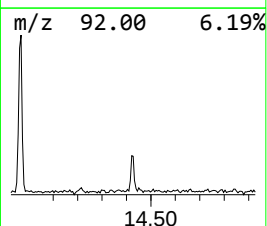
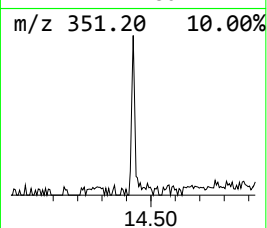
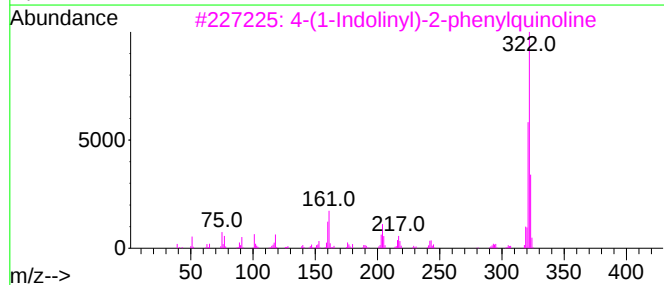
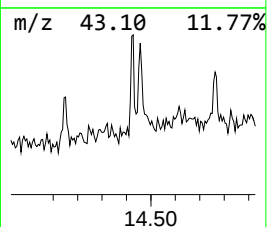
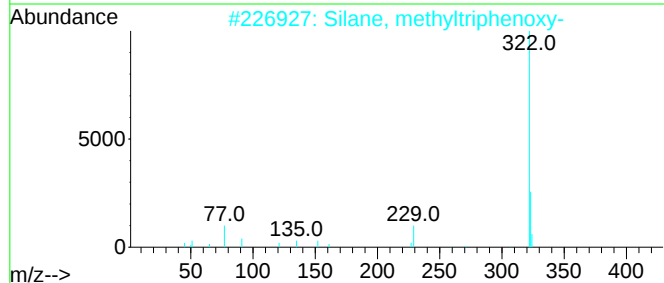
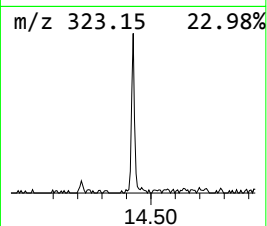
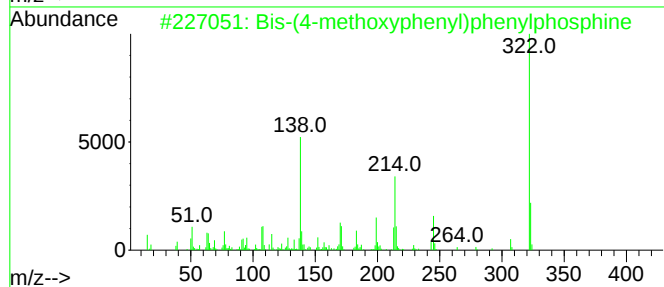
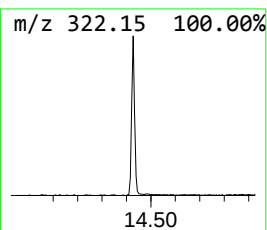
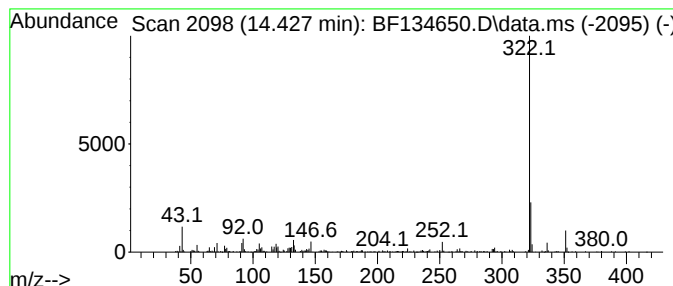
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bis-(4-methoxyphenyl)phenyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	2.00 ng	136991	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis-(4-methoxyphenyl)phenylphosp...	322	C20H19O2P	014180-51-9	59
2			Silane, methyltriphenoxy-	322	C19H18O3Si	003439-97-2	59
3			4-(1-Indolinyl)-2-phenylquinoline	322	C23H18N2	1000326-78-8	59
4			(1S)-7-methoxy-1-methyl-1,2,3,4-...	337	C17H31N02Si2	1000472-33-0	59
5			Phenol, 2-(2H-benzotriazol-2-yl)...	351	C22H29N3O	025973-55-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134650.D
Acq On : 07 Aug 2023 12:58
Operator : CG\JU
Sample : 03887-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MCLEAN-TP6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzenesulfonam...	10.475	3.8	ng	323058	3	9.833	1706460	20.0
Benzophenone	10.545	4.4	ng	375513	3	9.833	1706460	20.0
Benzenesulfonam...	10.675	11.4	ng	845481	4	11.322	1483100	20.0
n-Hexadecanoic ...	11.857	3.3	ng	247837	4	11.322	1483100	20.0
1-Heneicosanol	13.821	5.2	ng	355757	5	13.968	1367510	20.0
Bis-(4-methoxyp...	14.427	2.0	ng	136991	5	13.968	1367510	20.0