

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
 Data File : BF134632.D
 Acq On : 04 Aug 2023 14:52
 Operator : CG\JU
 Sample : 03887-01
 Misc :
 ALS Vial : 13 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: BF134632.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.887	301	306	311	rVB	83226	109203	3.46%	0.445%
2	5.034	497	501	507	rVB	45160	51274	1.63%	0.209%
3	5.428	563	568	571	rBV	3266419	3006288	95.32%	12.257%
4	6.428	733	738	741	rBV	2826221	3019128	95.72%	12.309%
5	6.798	797	801	804	rBV	1446132	1084564	34.39%	4.422%
6	7.357	891	896	899	rBV	2172417	1894319	60.06%	7.723%
7	8.075	1014	1018	1021	rBV	1741078	1368884	43.40%	5.581%
8	9.151	1197	1201	1205	rBV	3541456	3154032	100.00%	12.859%
9	9.833	1313	1317	1320	rBV	1357224	1243914	39.44%	5.072%
10	10.475	1422	1426	1429	rBV	273971	215343	6.83%	0.878%
11	10.545	1435	1438	1441	rVB	333184	246506	7.82%	1.005%
12	10.616	1446	1450	1454	rBV	1604768	1440825	45.68%	5.874%
13	10.675	1456	1460	1463	rBV	734869	629502	19.96%	2.567%
14	11.316	1566	1569	1572	rBV	1109031	1027896	32.59%	4.191%
15	11.339	1572	1573	1577	rVV	68927	50437	1.60%	0.206%
16	11.392	1578	1582	1585	rVB	45175	41478	1.32%	0.169%
17	11.857	1657	1661	1666	rBV	232093	241657	7.66%	0.985%
18	12.533	1772	1776	1779	rBV	172890	146759	4.65%	0.598%
19	12.645	1792	1795	1799	rBV2	36422	39115	1.24%	0.159%
20	12.763	1809	1815	1818	rBV	145074	149234	4.73%	0.608%
21	12.916	1837	1841	1844	rBV	2908896	2635957	83.57%	10.747%
22	13.821	1991	1995	2004	rBV2	310064	337314	10.69%	1.375%
23	13.968	2015	2020	2023	rBV	1186999	1235904	39.18%	5.039%
24	13.992	2023	2024	2026	rVB	70701	36079	1.14%	0.147%
25	14.210	2059	2061	2066	rBV	44647	48878	1.55%	0.199%
26	14.427	2095	2098	2101	rBV	131483	136074	4.31%	0.555%
27	15.004	2193	2196	2206	rVB	62248	124432	3.95%	0.507%
28	15.368	2255	2258	2262	rVB	44947	50111	1.59%	0.204%
29	15.433	2264	2269	2274	rBV	622226	762420	24.17%	3.108%

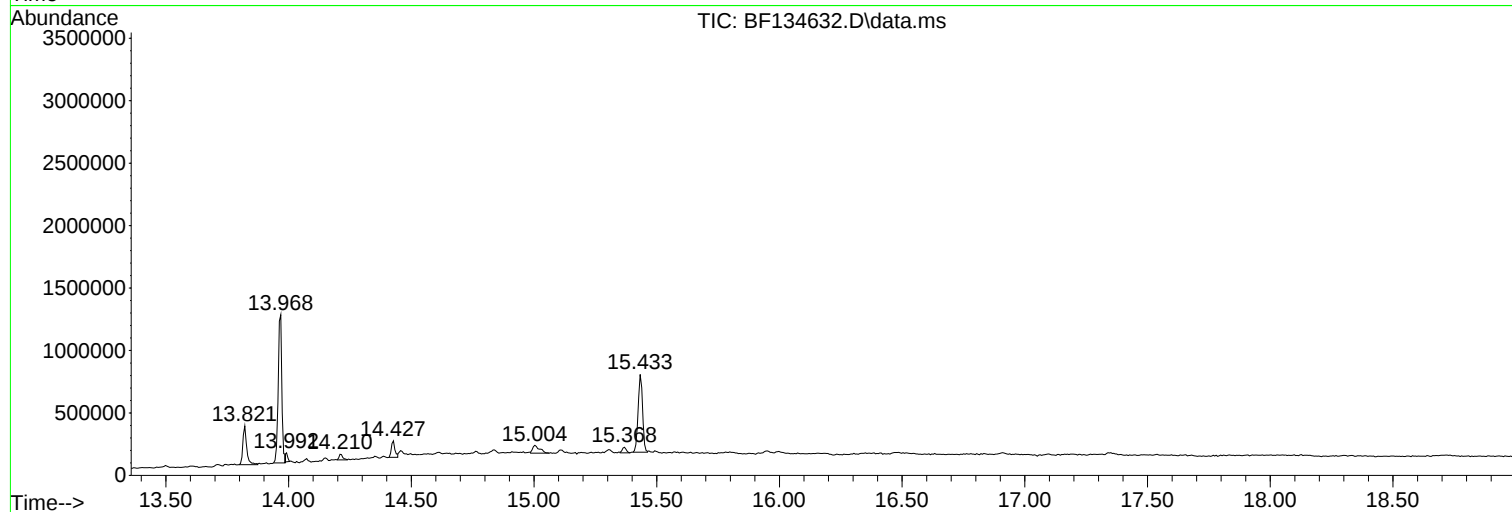
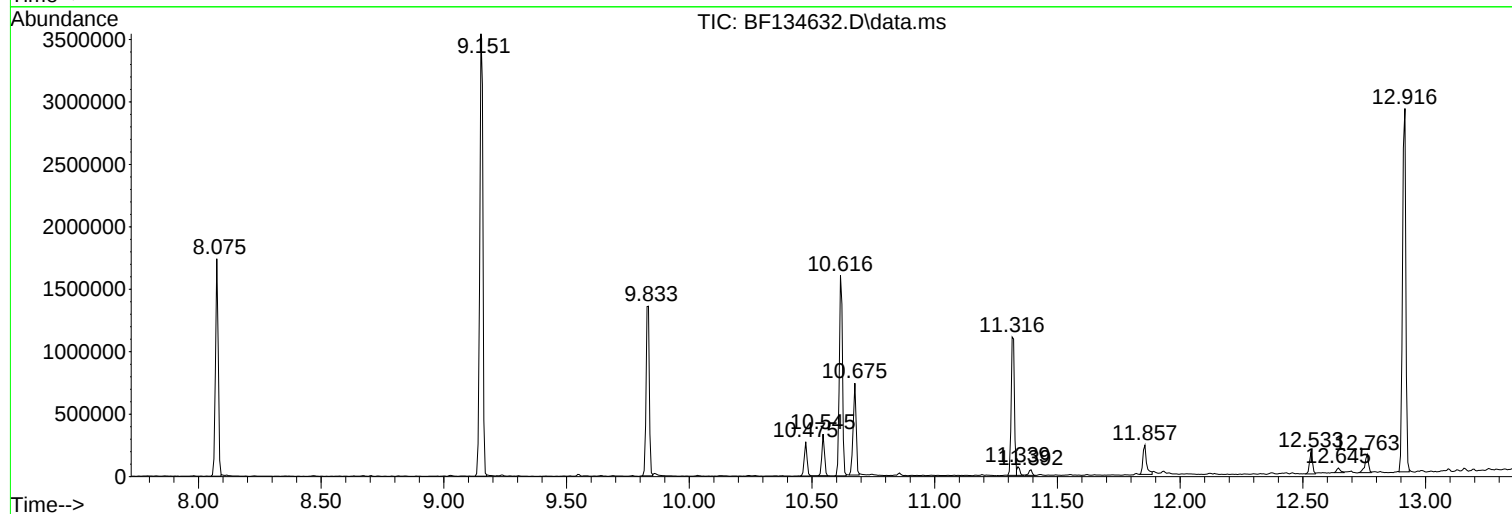
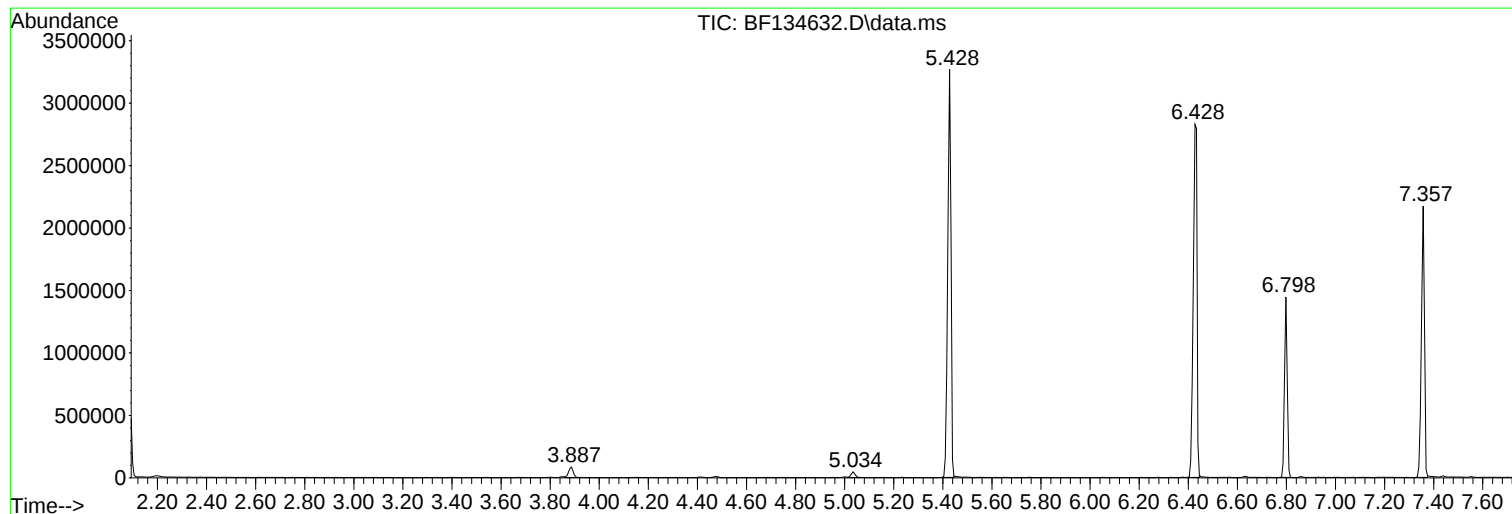
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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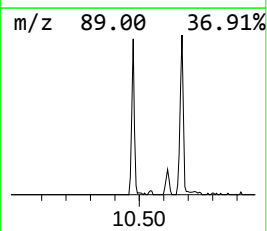
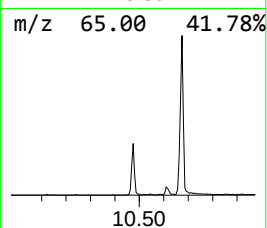
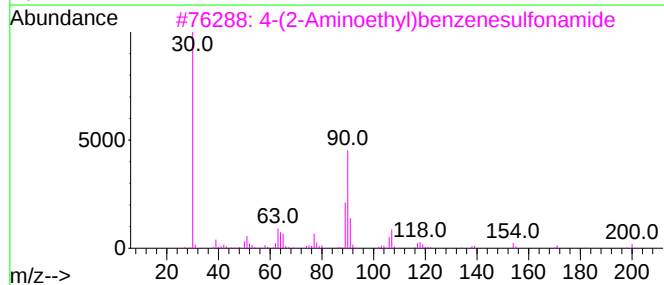
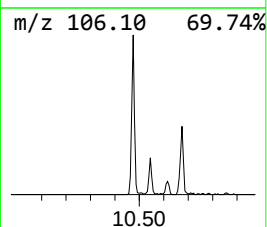
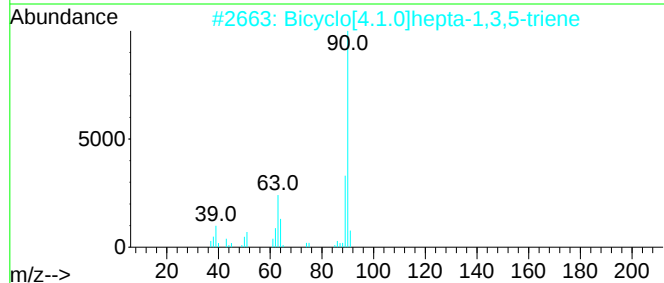
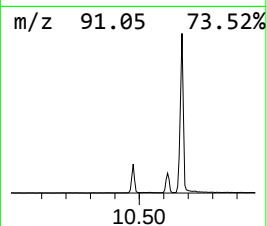
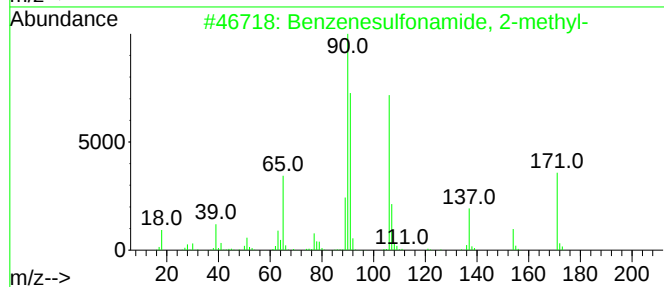
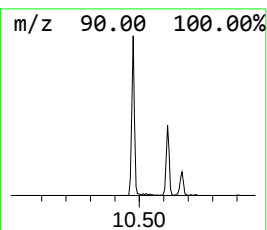
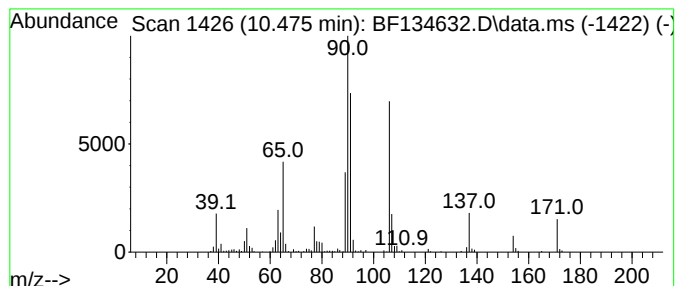
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzenesulfonamide, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.46 ng	215343	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	96
2			Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	47
3			4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	28
4			3,5-Octadiyne	106	C8H10	016387-70-5	27
5			Gluconic acid	196	C6H12O7	000526-95-4	23



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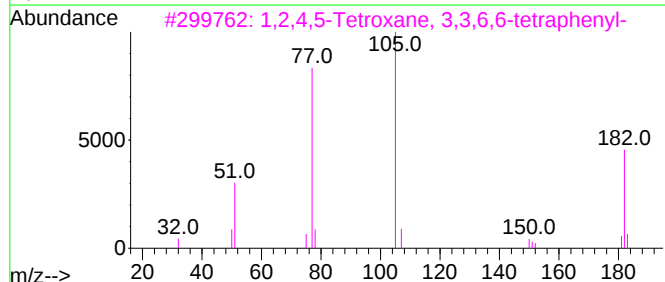
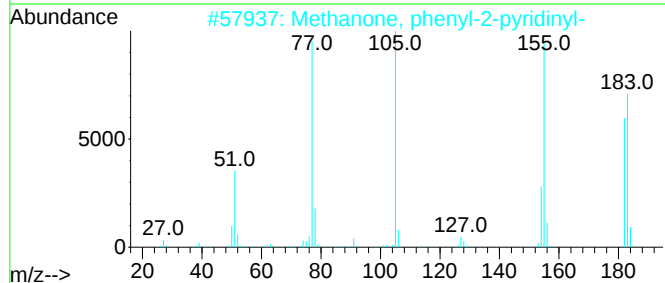
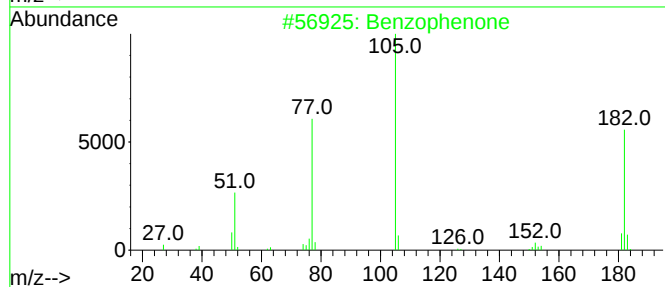
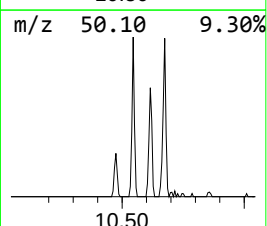
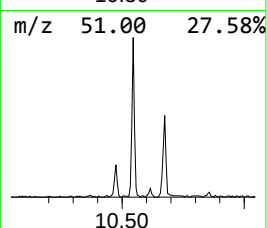
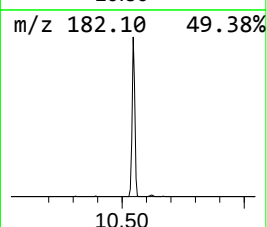
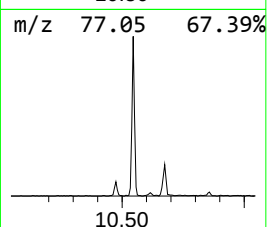
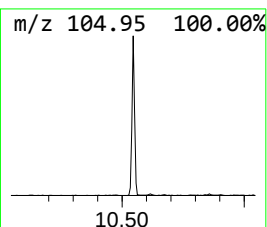
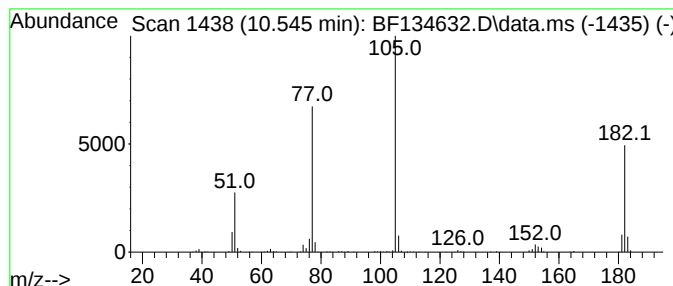
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Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.545	3.96 ng	246506	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	78
3			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	50
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	50



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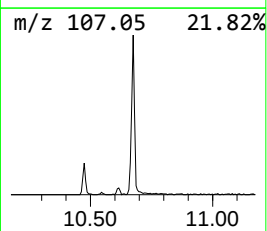
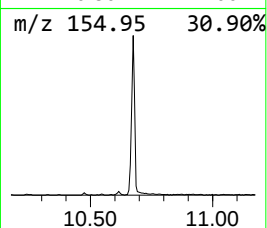
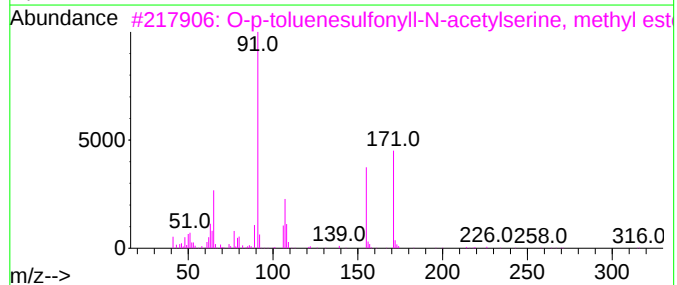
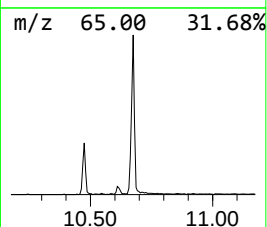
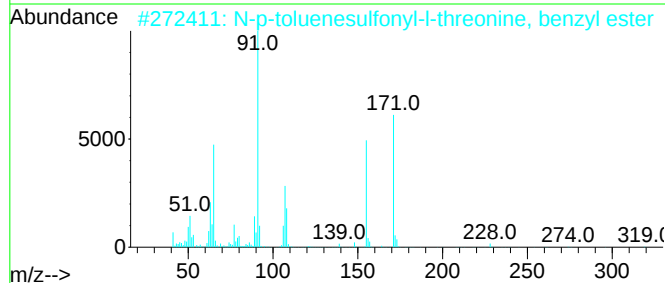
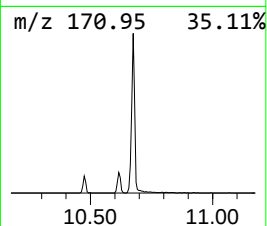
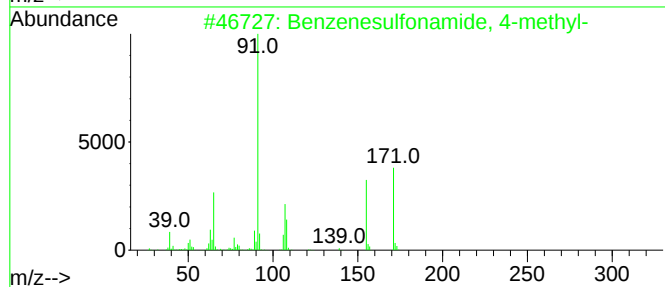
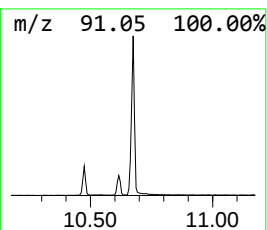
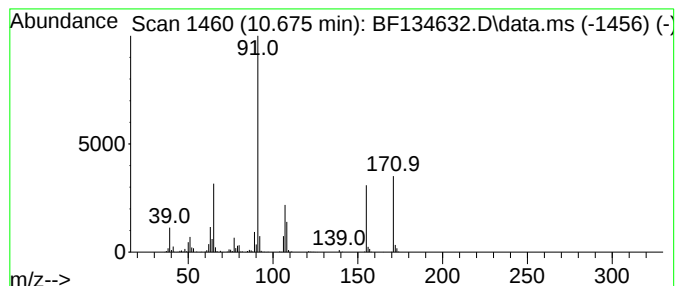
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Peak Number 4 Benzenesulfonamide, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.675	12.25 ng	629502	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			O-p-toluenesulfonyl-L-N-acetylser...	315	C13H17NO6S	1000126-44-8	59
4			4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	38
5			1-Hydroxytricyclo[4.3.0.0(4,9)]n...	308	C16H20O4S	201992-83-8	38



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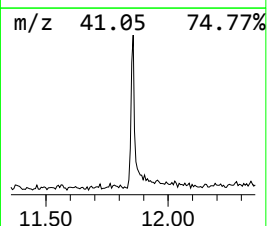
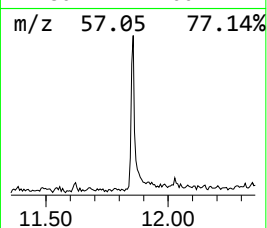
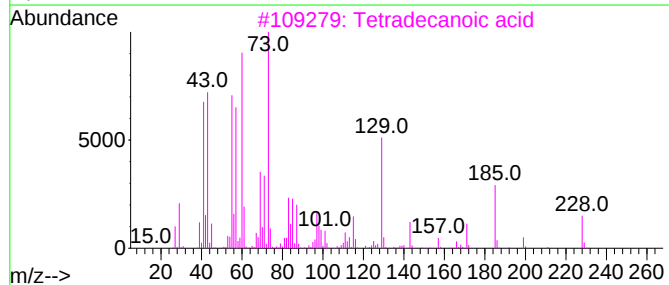
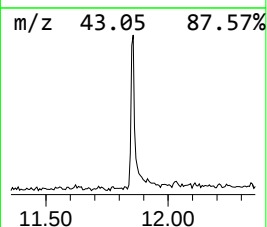
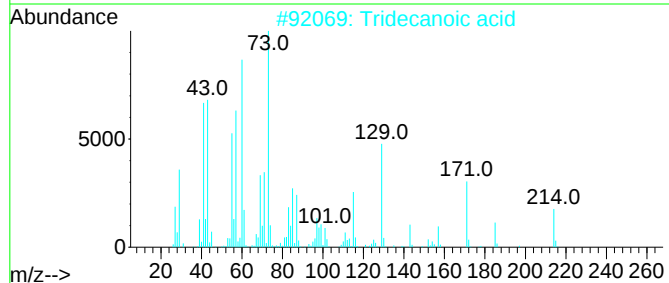
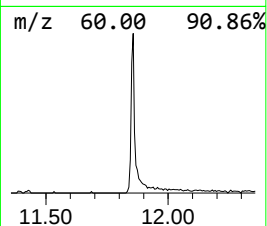
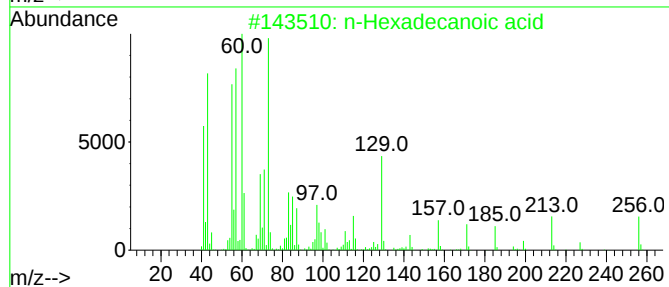
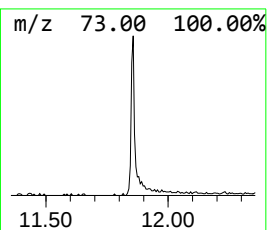
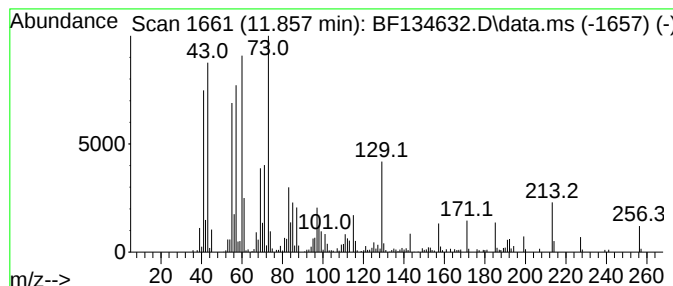
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.70 ng	241657	Phenanthrene-d10	11.322

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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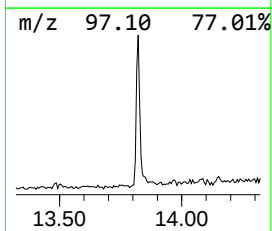
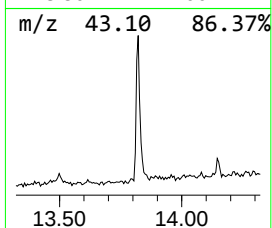
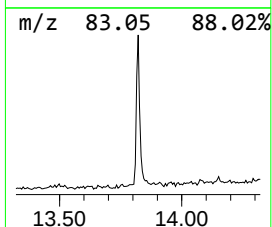
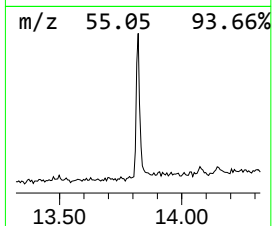
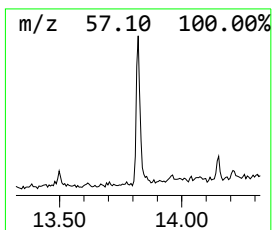
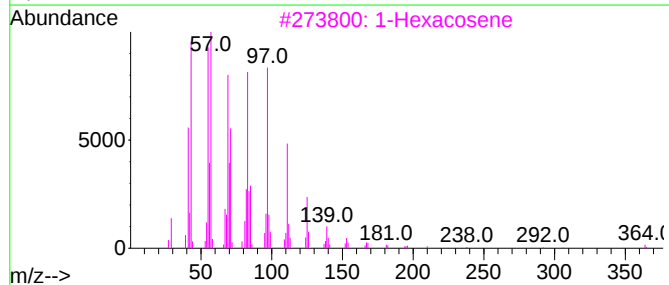
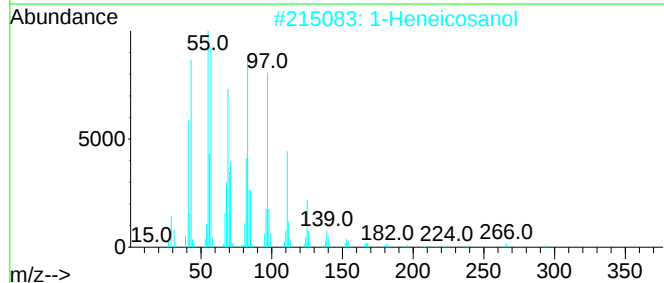
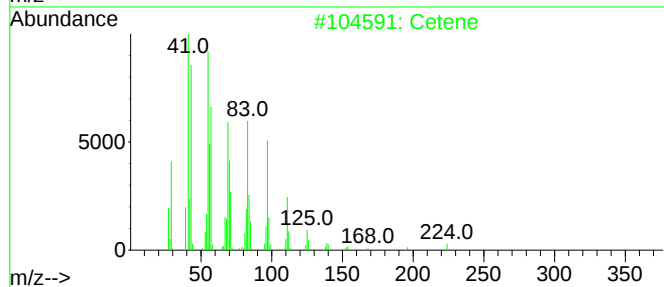
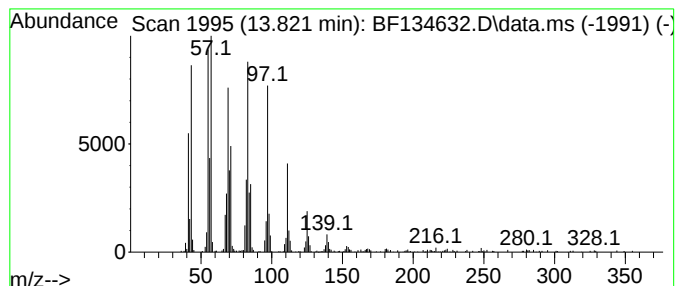
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Peak Number 7 Cetene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	5.46 ng	337314	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cetene	224	C16H32	000629-73-2	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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MCLEAN-TP6

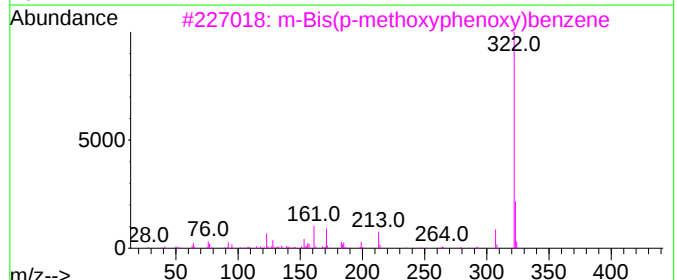
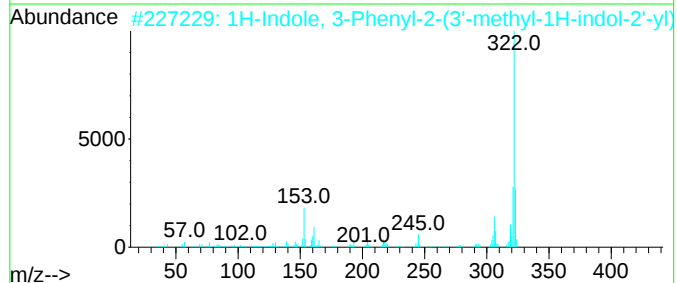
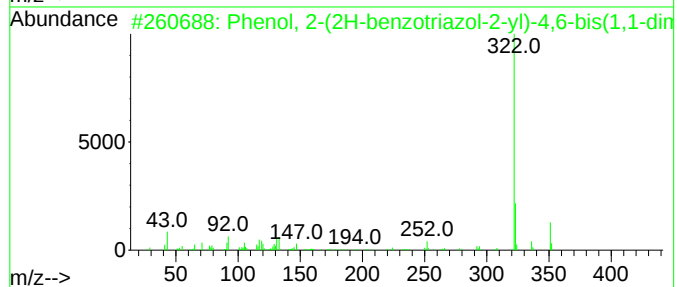
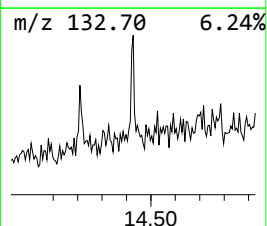
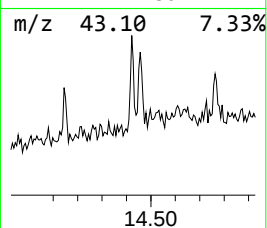
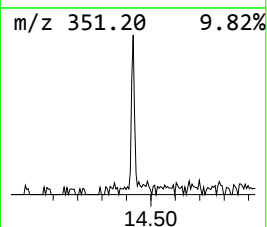
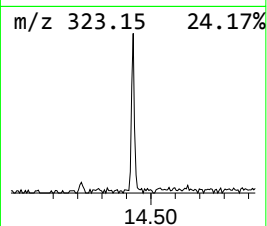
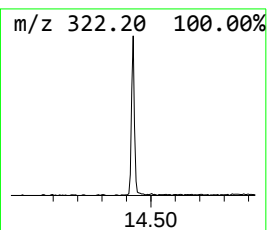
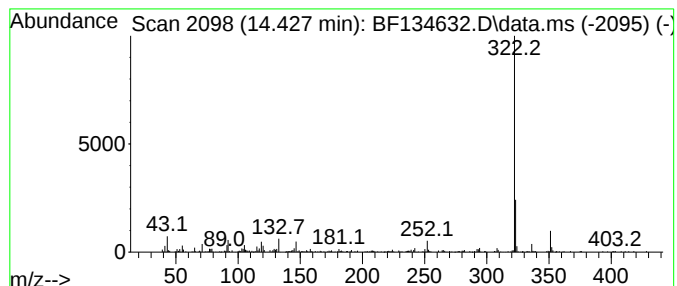
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 2-(2H-benzotriazol-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	2.20 ng	136074	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(2H-benzotriazol-2-yl)...	351	C22H29N3O	025973-55-1	90
2			1H-Indole, 3-Phenyl-2-(3'-methyl...	322	C23H18N2	164936-86-1	64
3			m-Bis(p-methoxyphenoxy)benzene	322	C20H18O4	013118-91-7	59
4			Carbonic acid, monoamide, N-(2-p...	365	C23H43N02	1010490-04-9	59
5			1-Methyl-2,6-diphenyl-4,4-pentam...	365	C25H23N3	083078-31-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
Data File : BF134632.D
Acq On : 04 Aug 2023 14:52
Operator : CG\JU
Sample : 03887-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MCLEAN-TP6

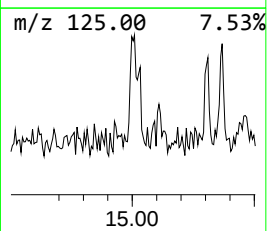
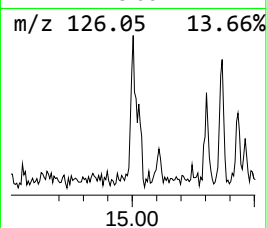
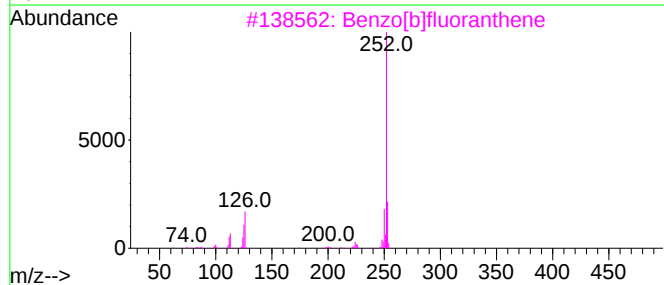
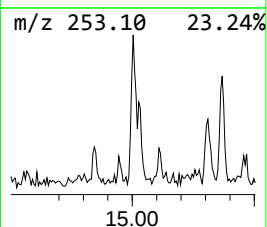
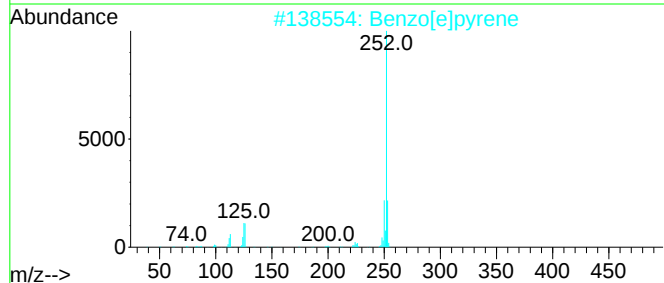
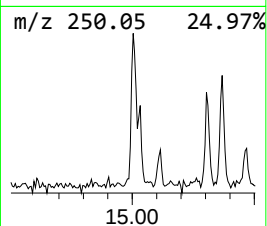
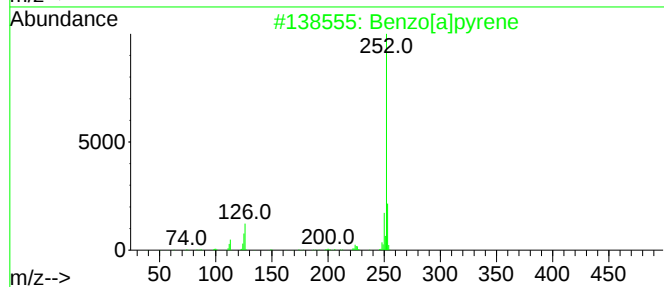
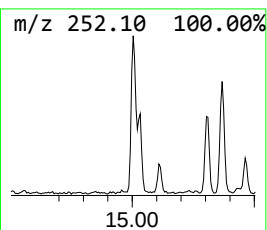
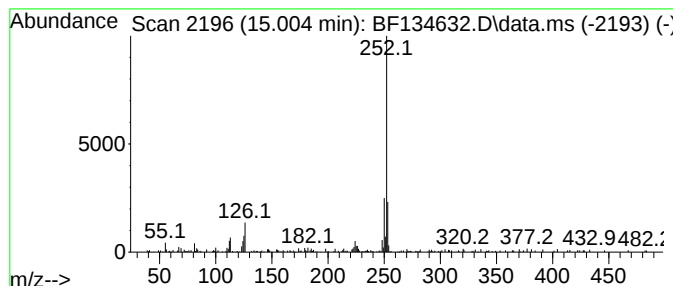
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	3.26 ng	124432	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	94
2			Benzo[e]pyrene	252	C20H12	000192-97-2	90
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080423\
Data File : BF134632.D
Acq On : 04 Aug 2023 14:52
Operator : CG\JU
Sample : 03887-01
Misc :
ALS Vial : 13 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzenesulfonam...	10.475	3.5	ng	215343	3	9.833	1243910	20.0
Benzophenone	10.545	4.0	ng	246506	3	9.833	1243910	20.0
Benzenesulfonam...	10.675	12.3	ng	629502	4	11.322	1027900	20.0
n-Hexadecanoic ...	11.857	4.7	ng	241657	4	11.322	1027900	20.0
Cetene	13.821	5.5	ng	337314	5	13.968	1235900	20.0
Phenol, 2-(2H-b...	14.427	2.2	ng	136074	5	13.968	1235900	20.0
Benzo[e]pyrene	15.004	3.3	ng	124432	6	15.433	762420	20.0