

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
 Data File : BF135309.D
 Acq On : 18 Sep 2023 16:33
 Operator : CG\JU
 Sample : 04391-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-26-WEST-MAIN-STREET

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135309.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.757	279	284	288	rBV	30991	45048	1.23%	0.194%
2	5.387	557	561	572	rBV	1899411	1764888	48.02%	7.585%
3	6.398	729	733	744	rBV	1220982	1149024	31.26%	4.938%
4	6.687	778	782	790	rBV	52653	63723	1.73%	0.274%
5	6.757	790	794	797	rBV	846598	697245	18.97%	2.997%
6	7.322	885	890	893	rVB	2272876	2245417	61.09%	9.650%
7	7.551	926	929	938	rVB2	64500	70582	1.92%	0.303%
8	7.716	952	957	961	rVB	1135664	1208192	32.87%	5.192%
9	7.775	961	967	970	rVV2	69487	78664	2.14%	0.338%
10	7.816	970	974	978	rVV	1702508	1595675	43.41%	6.858%
11	7.845	978	979	986	rVB2	66003	48980	1.33%	0.211%
12	8.034	1007	1011	1022	rVB	1093717	1000733	27.23%	4.301%
13	8.316	1053	1059	1062	rBV	104790	107680	2.93%	0.463%
14	9.116	1189	1195	1198	rBV	3923177	3675496	100.00%	15.796%
15	9.792	1304	1310	1313	rBV	1213912	1000376	27.22%	4.299%
16	9.898	1322	1328	1333	rBV	44417	46422	1.26%	0.200%
17	9.992	1341	1344	1353	rVB4	35275	53053	1.44%	0.228%
18	10.586	1441	1445	1449	rBV	2287442	2236704	60.85%	9.613%
19	10.892	1494	1497	1503	rBV	224270	201808	5.49%	0.867%
20	11.222	1550	1553	1558	rBV	51235	53337	1.45%	0.229%
21	11.286	1558	1564	1567	rBV	1189158	1074710	29.24%	4.619%
22	11.669	1624	1629	1634	rBV4	28125	49790	1.35%	0.214%
23	11.816	1649	1654	1663	rBV	291913	380719	10.36%	1.636%
24	12.345	1741	1744	1748	rBV	50618	41168	1.12%	0.177%
25	12.610	1784	1789	1798	rBV	149991	209946	5.71%	0.902%
26	12.886	1831	1836	1839	rBV	3037947	2917522	79.38%	12.539%
27	13.839	1992	1998	2002	rBV10	32119	71905	1.96%	0.309%
28	13.939	2011	2015	2020	rBV	621200	548243	14.92%	2.356%
29	15.404	2259	2264	2269	rBV	490750	631218	17.17%	2.713%

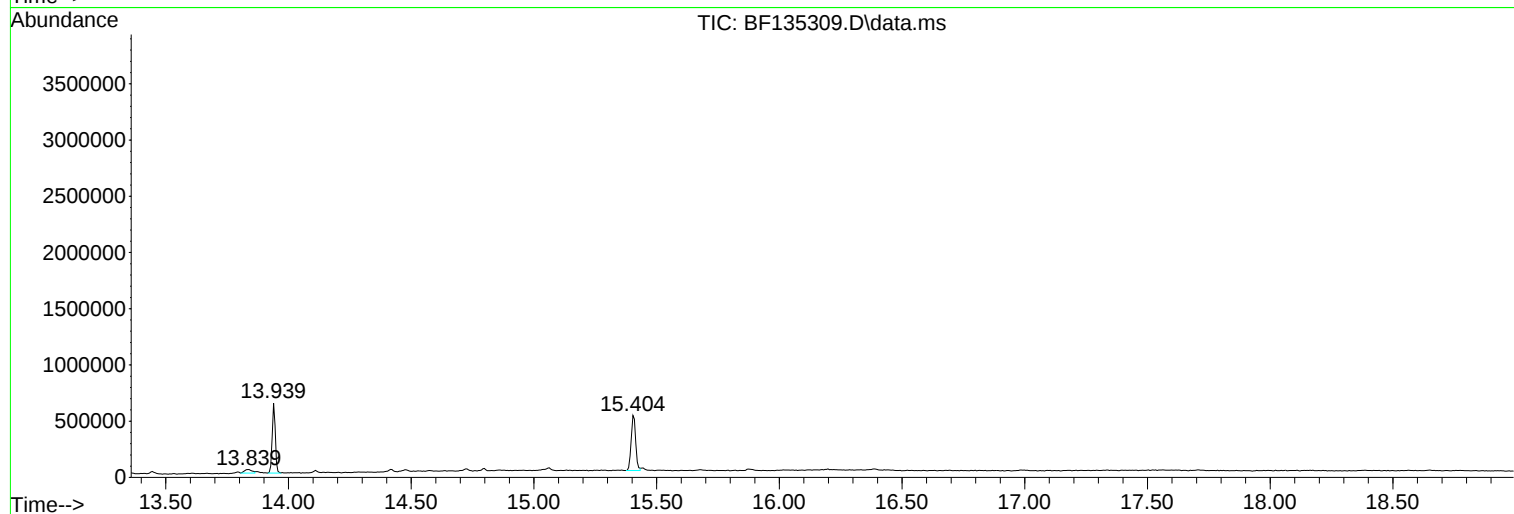
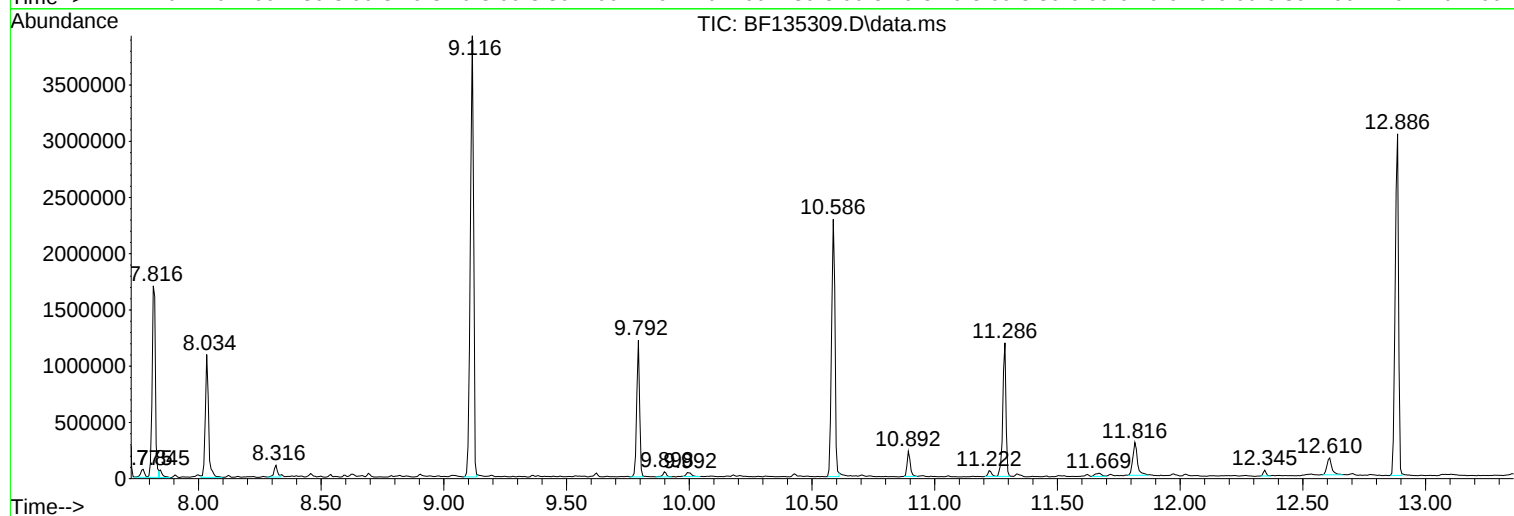
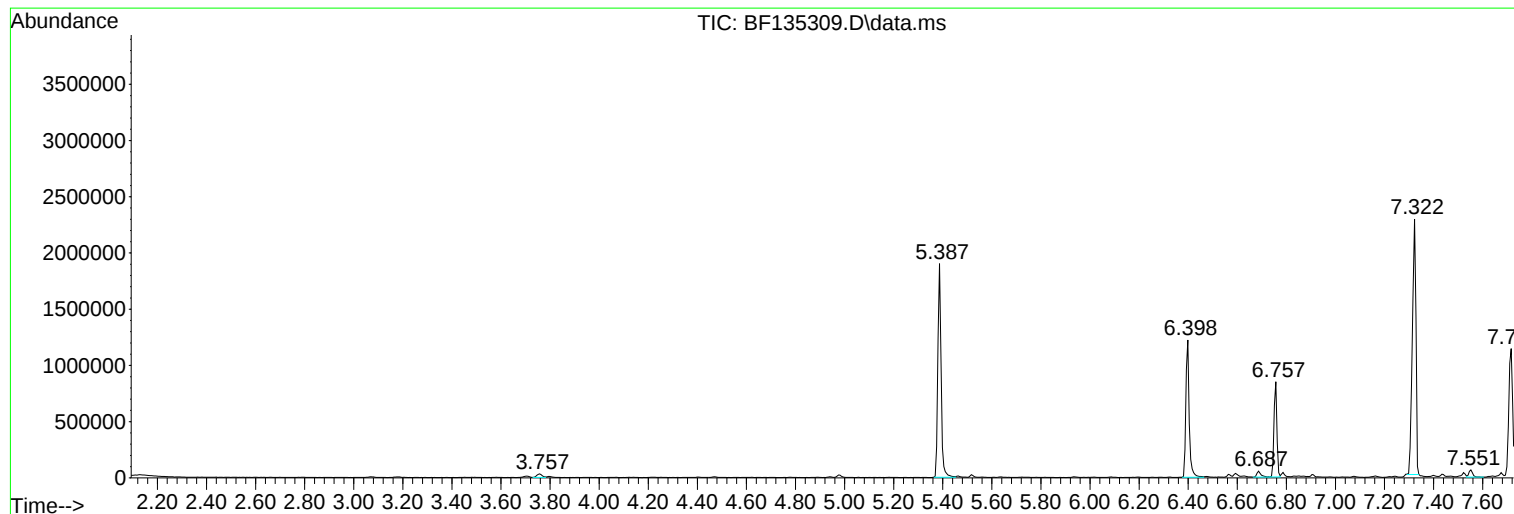
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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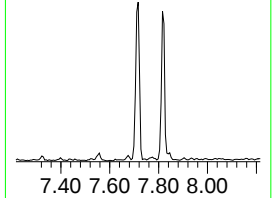
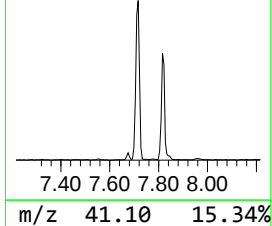
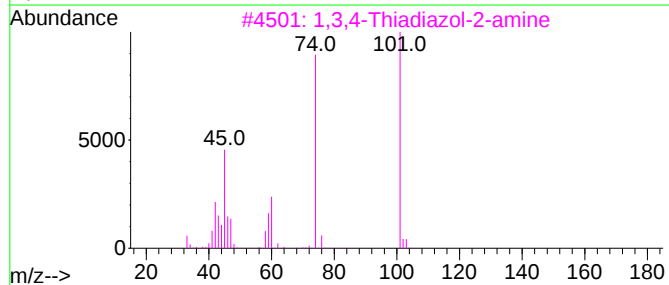
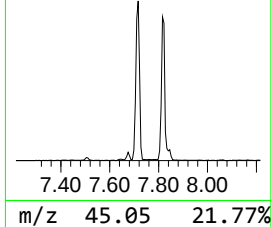
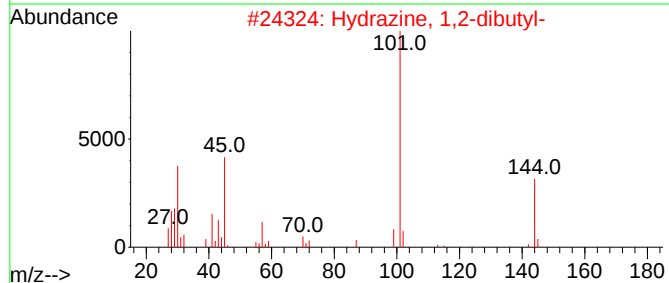
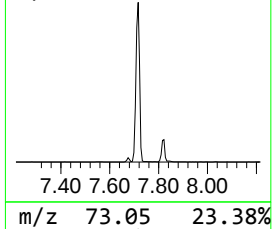
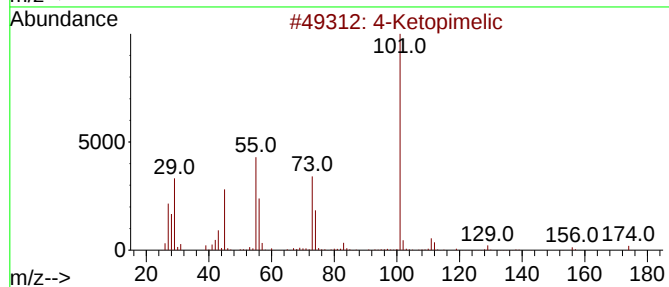
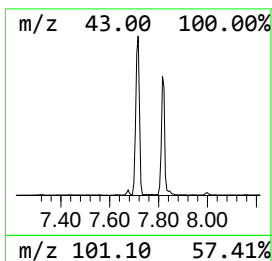
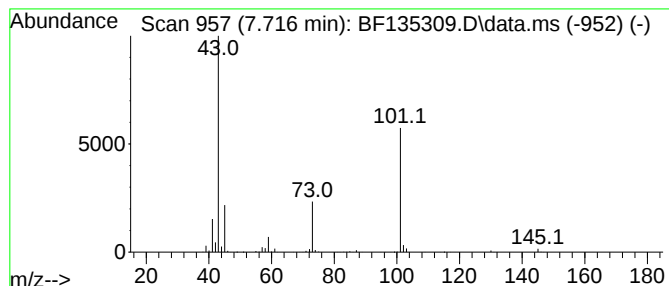
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 unknown7.716 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.716	24.15 ng	1208190	Naphthalene-d8	8.034

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Ketopimelic		174	C7H10O5	000502-50-1	42
2	Hydrazine, 1,2-dibutyl-		144	C8H20N2	001744-71-4	28
3	1,3,4-Thiadiazol-2-amine		101	C2H3N3S	004005-51-0	28
4	3H-1,2,4-Triazole-3-thione, 1,2-...		101	C2H3N3S	003179-31-5	25
5	Glutaric acid, di(4-methoxy-2-me...		332	C17H32O6	1010359-42-1	25



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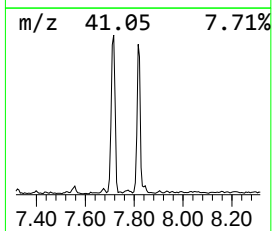
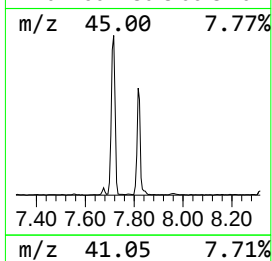
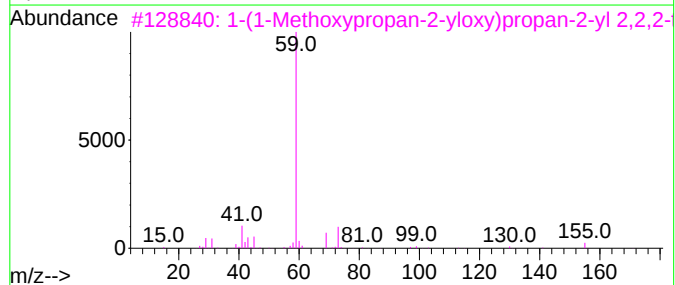
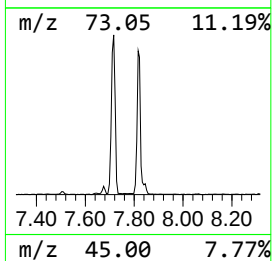
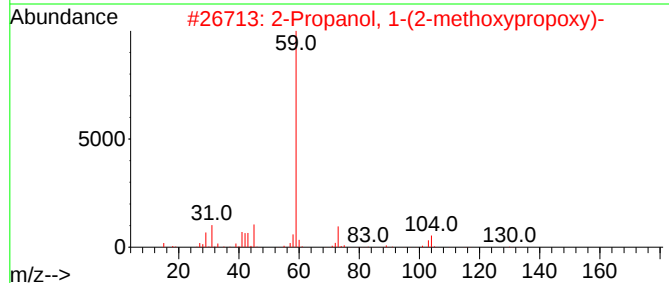
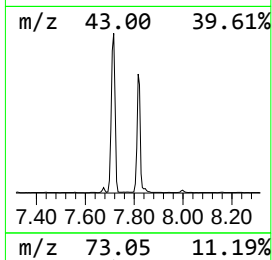
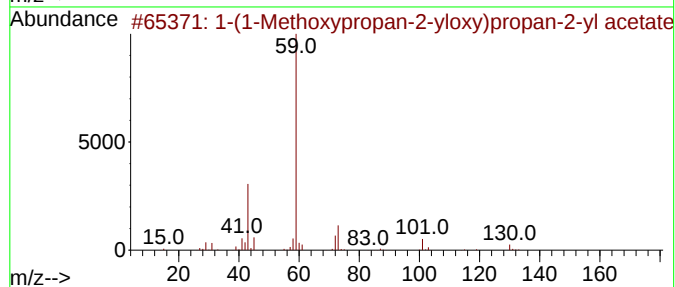
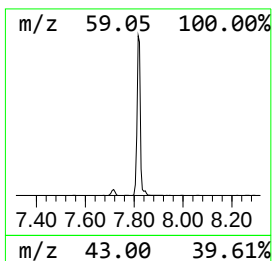
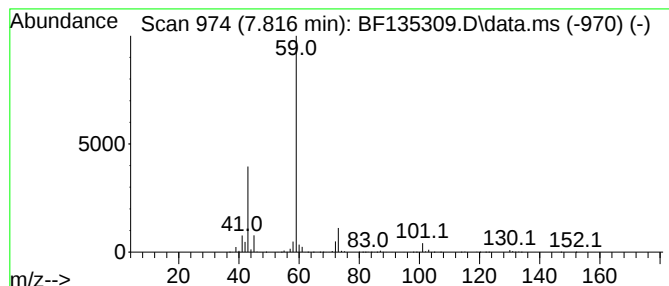
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Peak Number 2 1-(1-Methoxypropan-2-yloxy)... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.816	31.89 ng	1595680	Naphthalene-d8	8.034

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-Methoxypropan-2-yloxy)propa...	190	C9H18O4		1000367-08-6	83
2	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3		013429-07-7	72
3	1-(1-Methoxypropan-2-yloxy)propa...	244	C9H15F3O4		1010367-08-7	72
4	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3		020324-32-7	59
5	2-Hexanol, methyl ether	116	C7H16O		1000333-92-0	59



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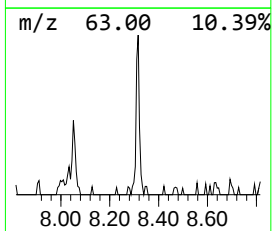
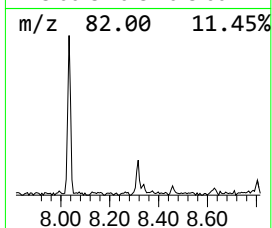
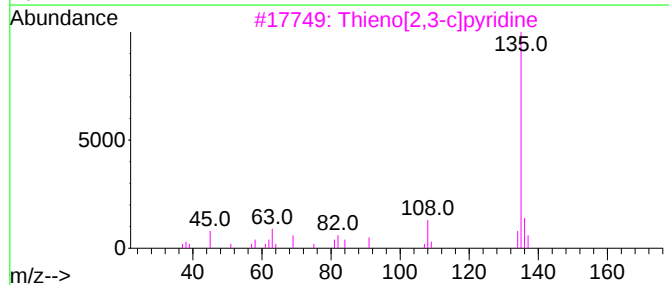
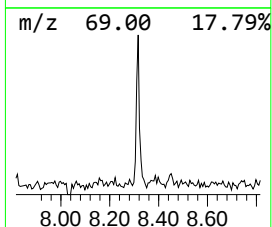
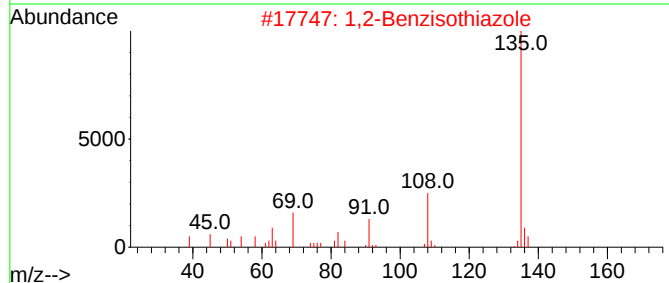
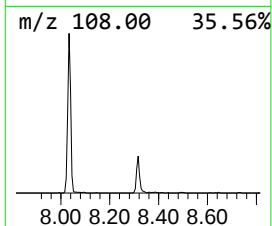
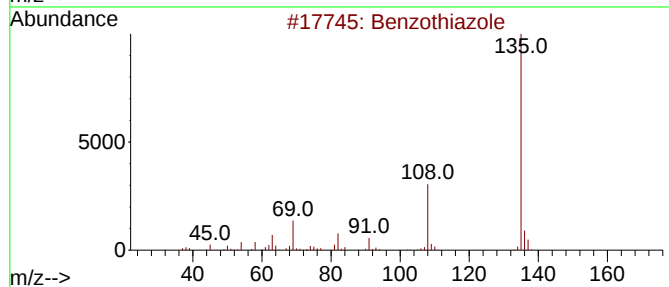
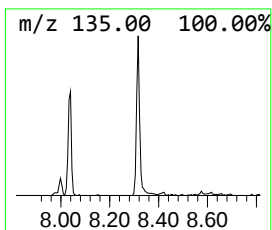
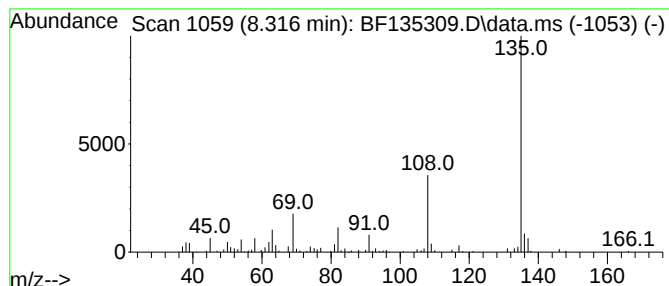
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Peak Number 3 Benzothiazole Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.316	2.15 ng	107680	Naphthalene-d8	8.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzothiazole	135	C7H5NS	000095-16-9	95
2			1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3			Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
4			2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64
5			3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	64



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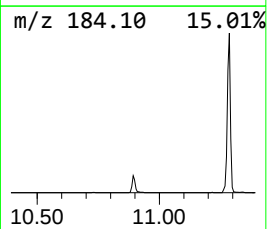
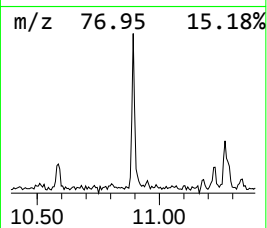
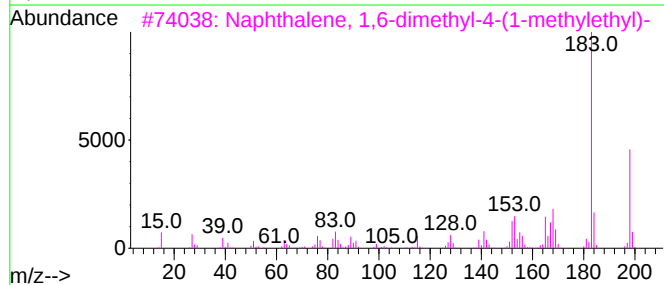
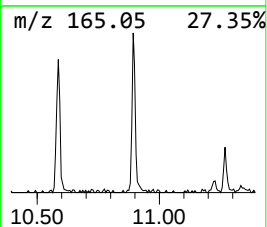
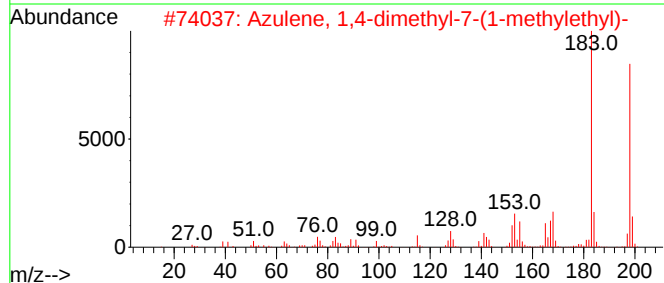
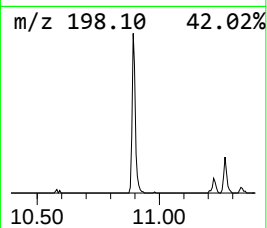
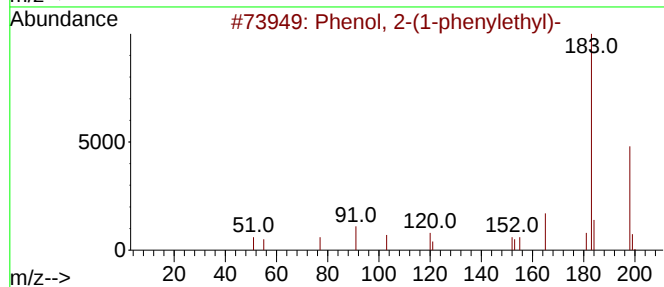
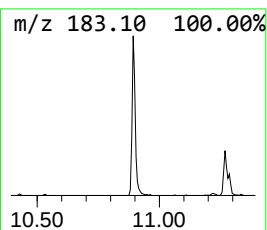
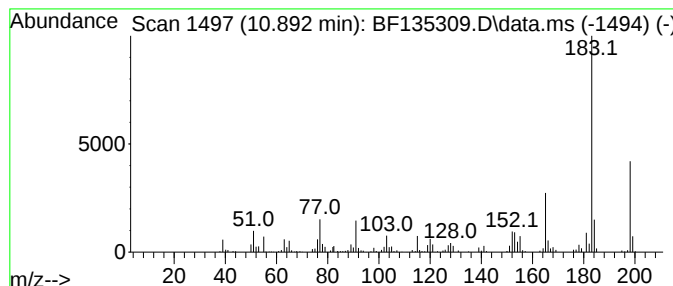
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Peak Number 4 Phenol, 2-(1-phenylethyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.892	3.76 ng	201808	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1-phenylethyl)-	198	C14H14O	004237-44-9	95
2			Azulene, 1,4-dimethyl-7-(1-methy...	198	C15H18	000489-84-9	90
3			Naphthalene, 1,6-dimethyl-4-(1-m...	198	C15H18	000483-78-3	90
4			Phenol, 4-(1-phenylethyl)-	198	C14H14O	001988-89-2	87
5			6-Isopropyl-1,4-dimethylnaphthalene	198	C15H18	000489-77-0	80



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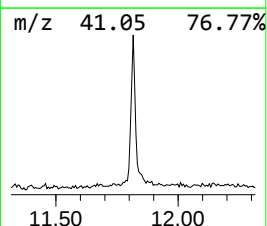
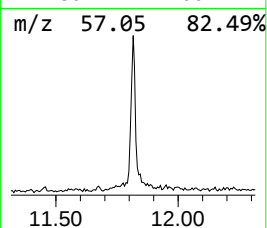
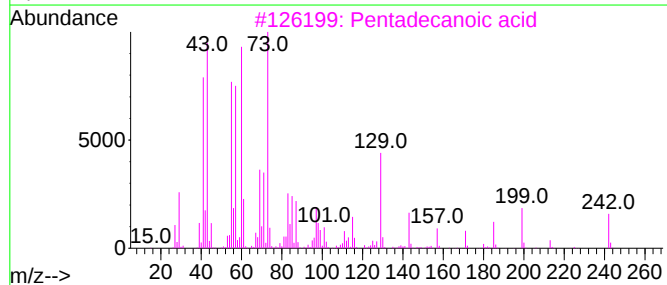
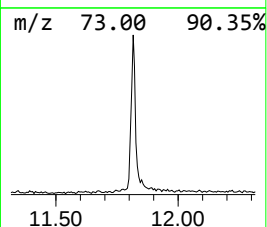
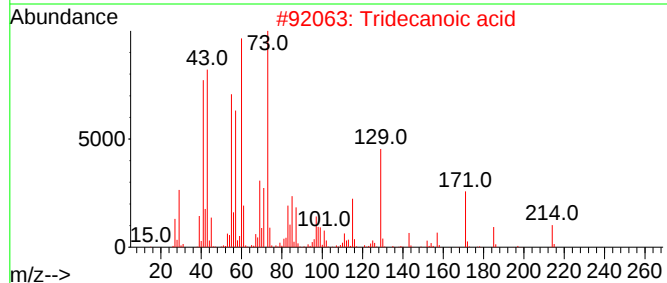
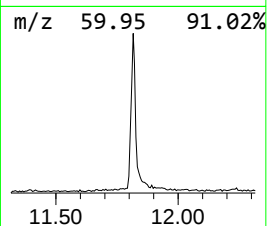
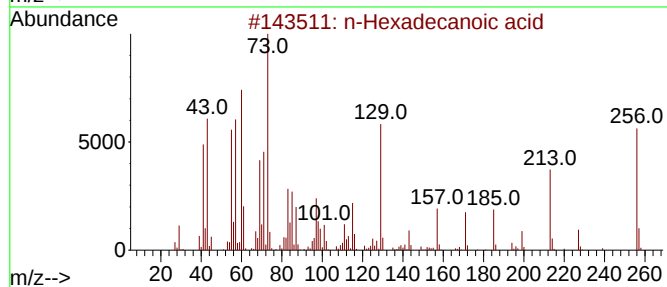
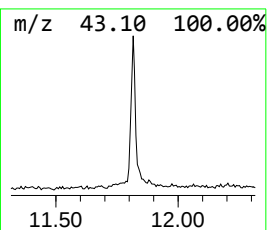
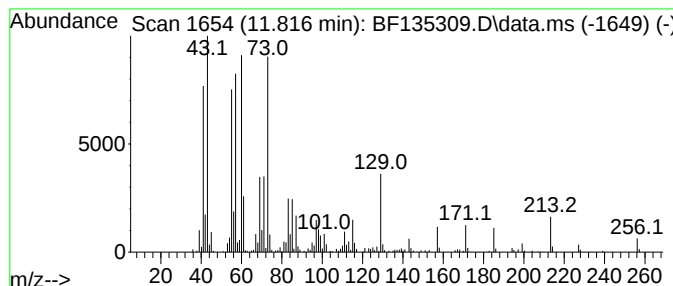
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	7.09 ng	380719	Phenanthrene-d10	11.286

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	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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ClientSampleId :
GW-26-WEST-MAIN-STREET

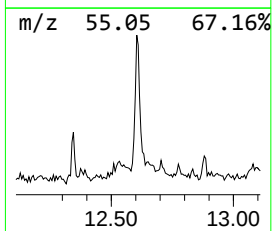
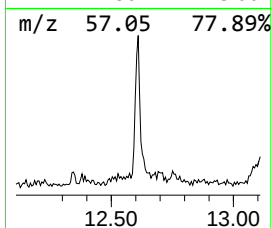
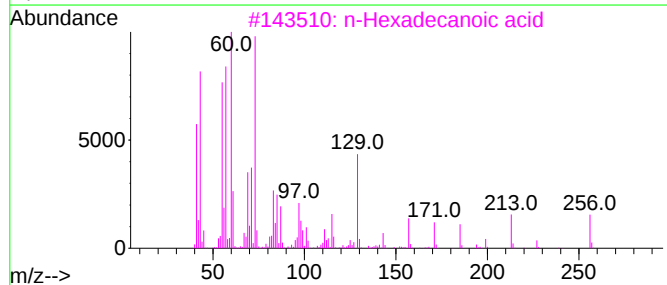
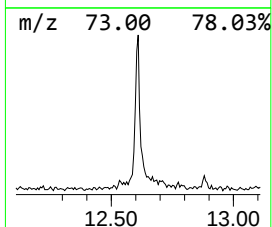
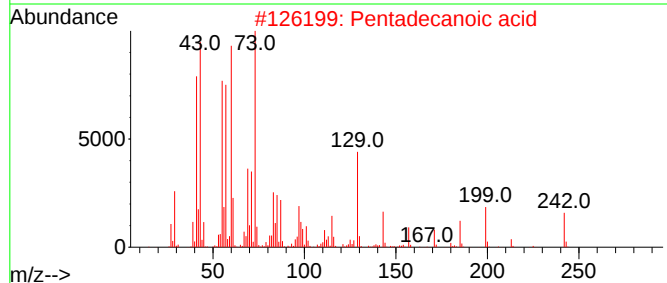
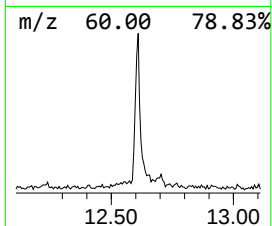
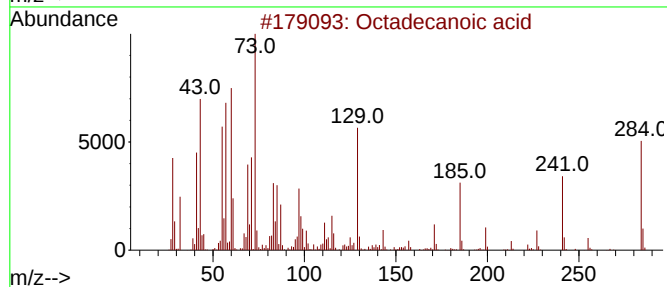
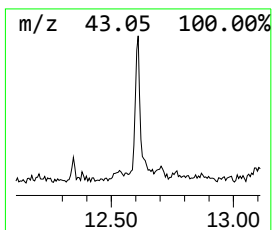
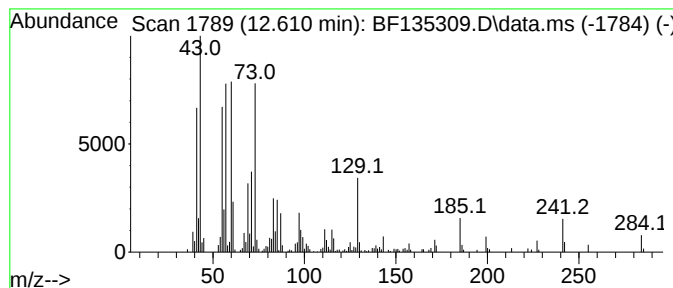
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.610	3.91 ng	209946	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
Data File : BF135309.D
Acq On : 18 Sep 2023 16:33
Operator : CG\JU
Sample : 04391-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-26-WEST-MAIN-STREET

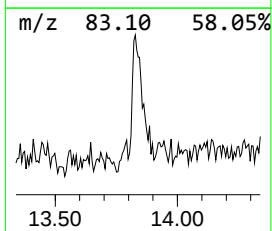
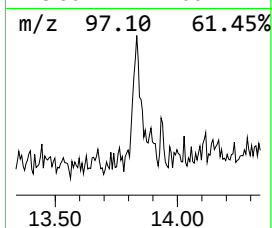
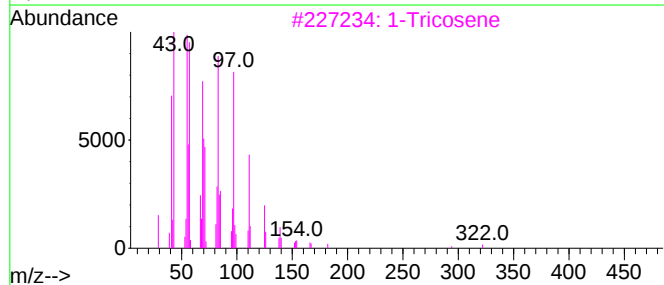
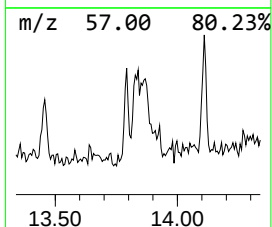
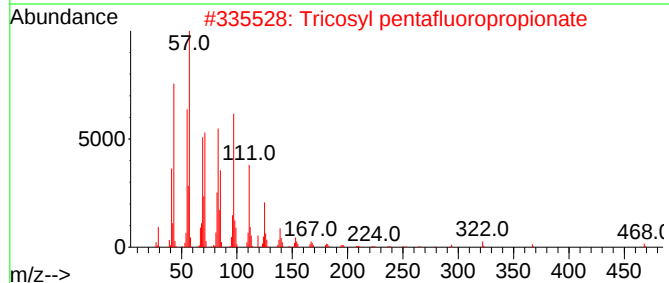
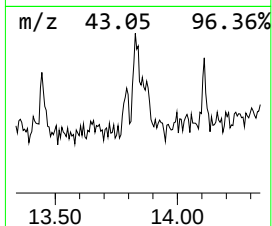
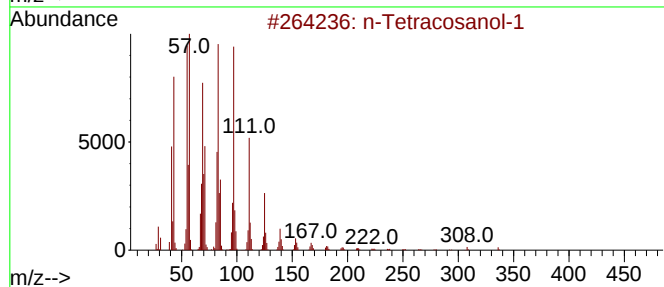
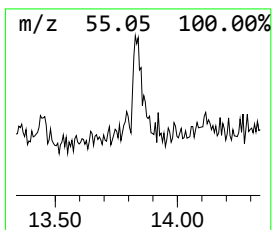
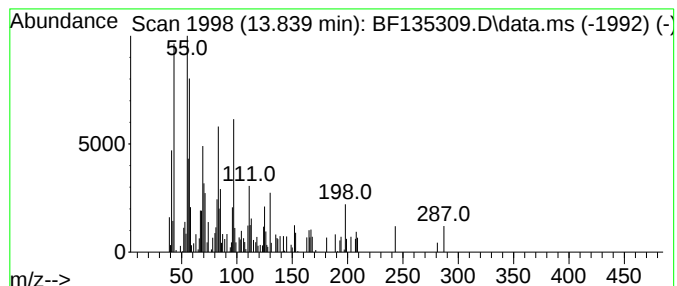
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	2.62 ng	71905	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	60
2			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	58
3			1-Tricosene	322	C23H46	018835-32-0	55
4			Acetic acid n-octadecyl ester	312	C20H40O2	000822-23-1	53
5			1-Heneicosanol	312	C21H44O	015594-90-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091823\
Data File : BF135309.D
Acq On : 18 Sep 2023 16:33
Operator : CG\JU
Sample : 04391-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-26-WEST-MAIN-STREET

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
unknown7.716	7.716	24.1	ng	1208190	2	8.034	1000730	20.0
1-(1-Methoxypro...	7.816	31.9	ng	1595680	2	8.034	1000730	20.0
Benzothiazole	8.316	2.1	ng	107680	2	8.034	1000730	20.0
Phenol, 2-(1-ph...	10.892	3.8	ng	201808	4	11.286	1074710	20.0
n-Hexadecanoic ...	11.816	7.1	ng	380719	4	11.286	1074710	20.0
Octadecanoic acid	12.610	3.9	ng	209946	4	11.286	1074710	20.0
n-Tetracosanol-1	13.839	2.6	ng	71905	5	13.939	548243	20.0