

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
 Data File : BF139554.D
 Acq On : 26 Sep 2024 18:59
 Operator : RC/JU
 Sample : P4176-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FB-1C-SYS2

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-BF091324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	3	11	17	rVB	2417353	3889886	100.00%	23.743%
2	5.081	500	508	516	rBV	106064	145380	3.74%	0.887%
3	5.493	573	578	587	rBV	628898	805382	20.70%	4.916%
4	6.504	744	750	762	rBV	496981	640626	16.47%	3.910%
5	6.875	808	813	818	rBV	368775	440464	11.32%	2.689%
6	7.440	902	909	914	rBV	1148710	1524220	39.18%	9.304%
7	8.157	1026	1031	1036	rBV	460554	555262	14.27%	3.389%
8	9.234	1208	1214	1219	rBV	1804377	2275977	58.51%	13.892%
9	9.910	1324	1329	1334	rBV	503463	613849	15.78%	3.747%
10	10.622	1445	1450	1458	rBV	78485	96468	2.48%	0.589%
11	10.698	1458	1463	1474	rBV	877809	1112317	28.60%	6.789%
12	11.192	1542	1547	1551	rBV	46098	53706	1.38%	0.328%
13	11.398	1576	1582	1591	rBV	511664	633435	16.28%	3.866%
14	11.922	1666	1671	1675	rBV	141232	215735	5.55%	1.317%
15	12.704	1799	1804	1817	rBV	36785	79684	2.05%	0.486%
16	12.980	1846	1851	1857	rBV	1858881	2470072	63.50%	15.077%
17	14.033	2023	2030	2037	rBV	300711	392998	10.10%	2.399%
18	14.657	2129	2136	2149	rVB5	23123	70433	1.81%	0.430%
19	15.510	2275	2281	2291	rBV	227008	367214	9.44%	2.241%

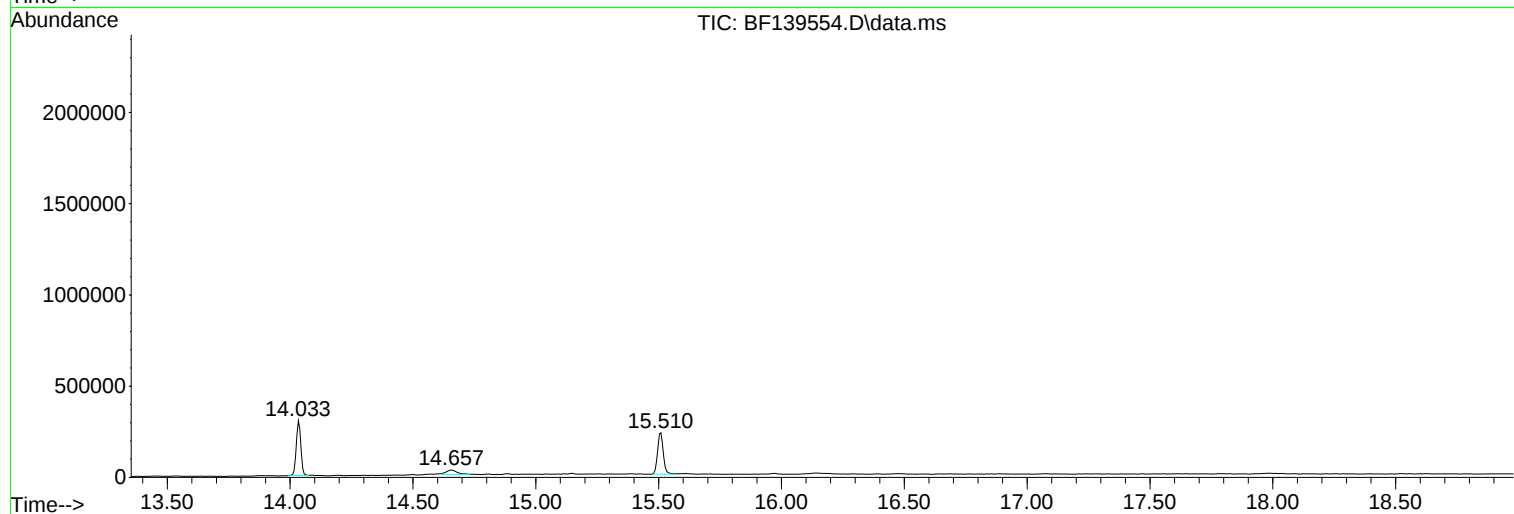
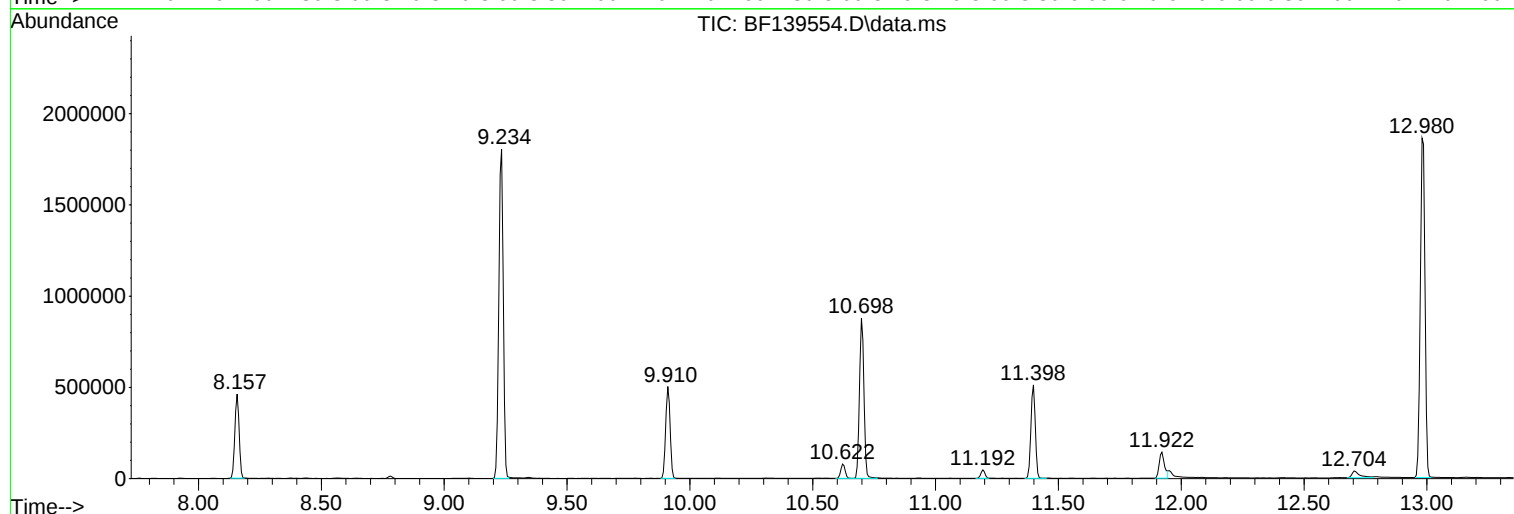
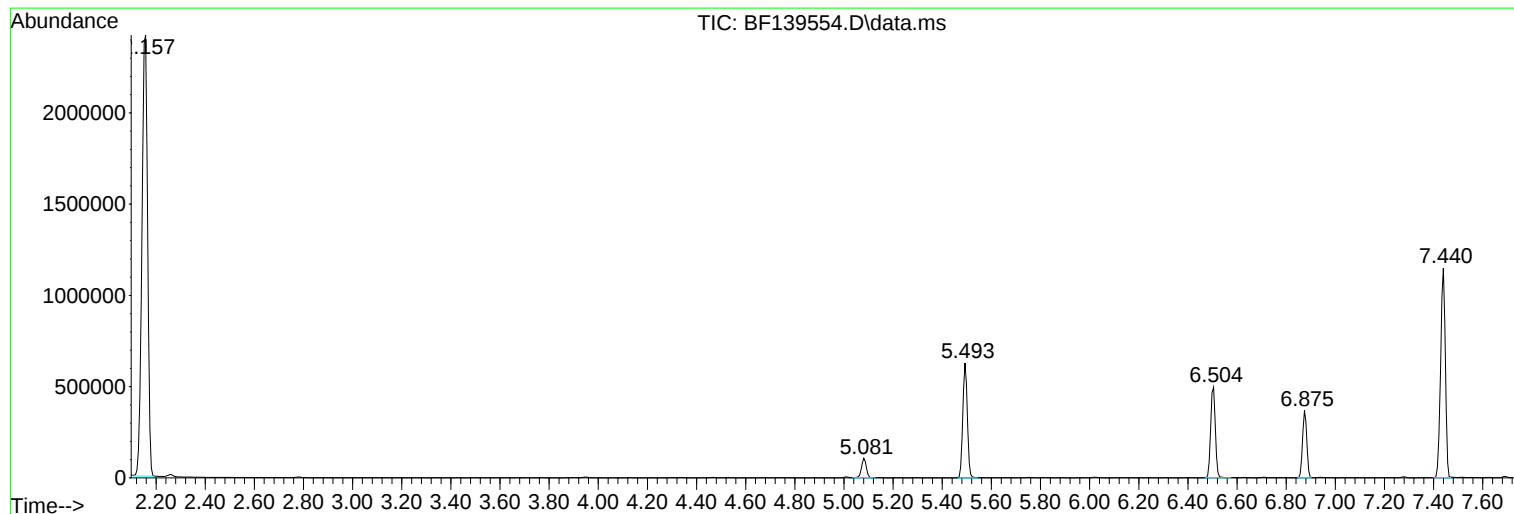
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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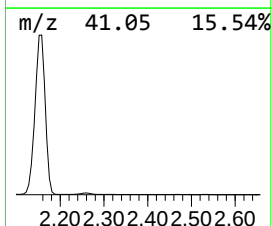
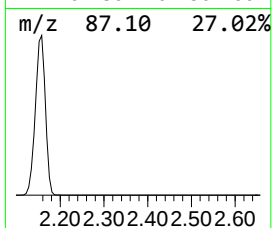
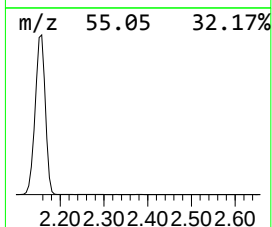
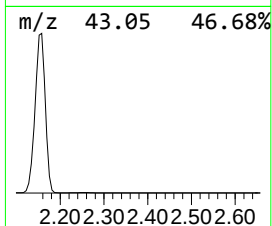
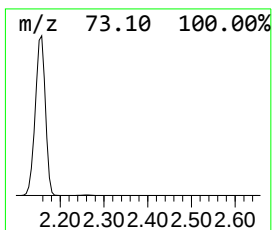
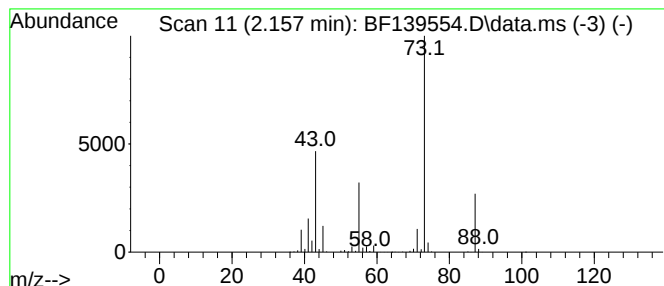
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	176.63 ng	3889890	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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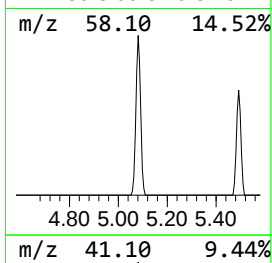
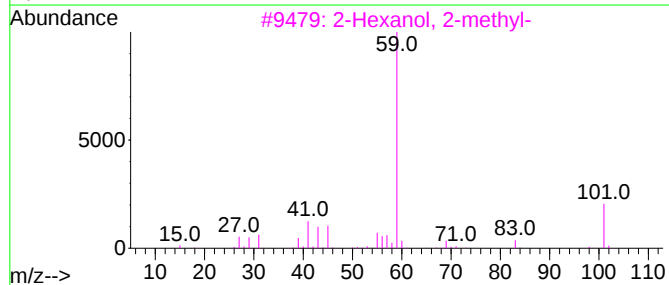
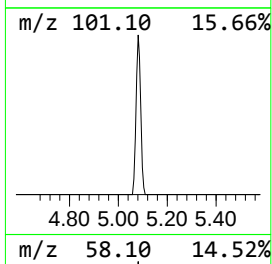
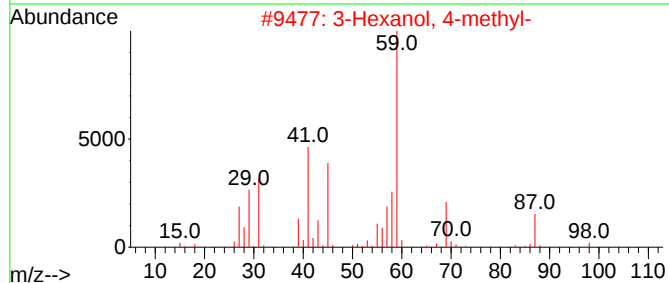
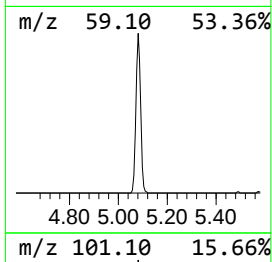
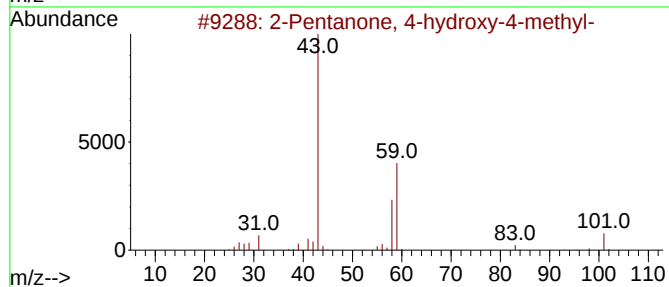
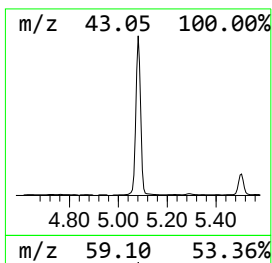
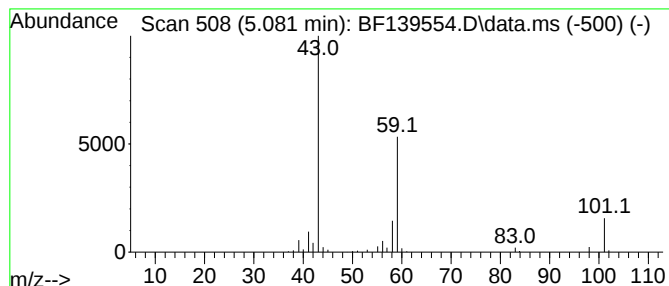
Instrument :
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ClientSampleId :
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.081	6.60 ng	145380	1,4-Dichlorobenzene-d4			6.875
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	28
4	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	28
5	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	25



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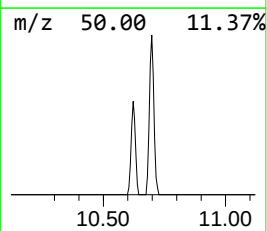
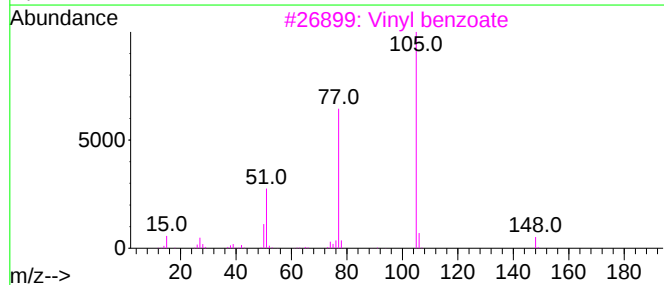
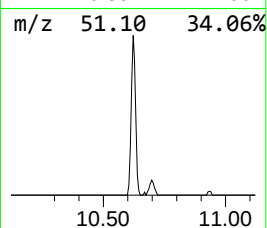
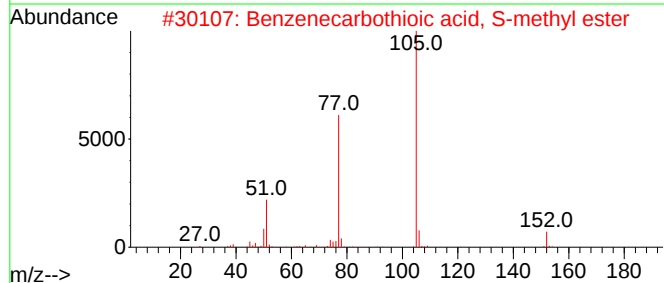
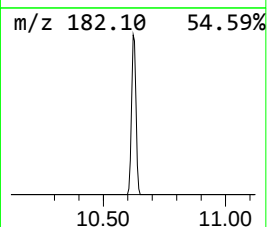
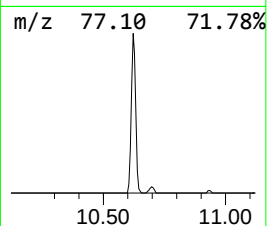
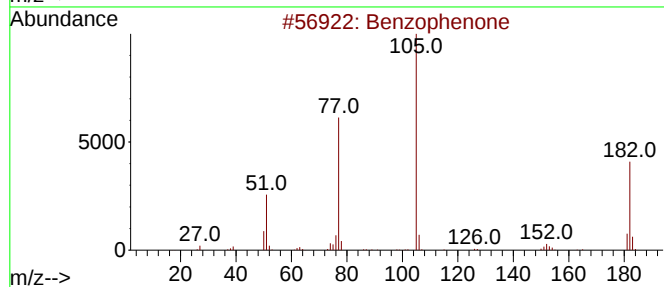
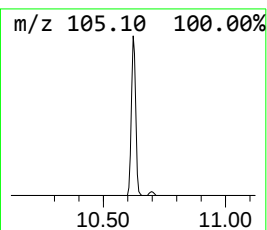
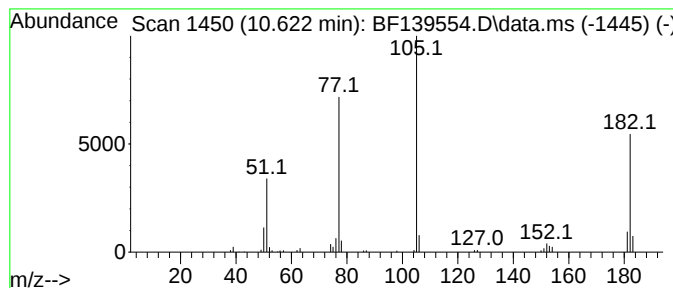
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	3.14 ng	96468	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			Propan-1-one, 3-nitro-1-phenyl-	179	C9H9NO3	062847-52-3	47
5			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47



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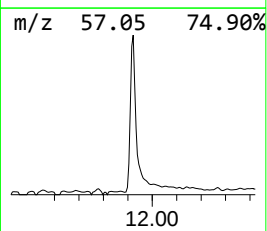
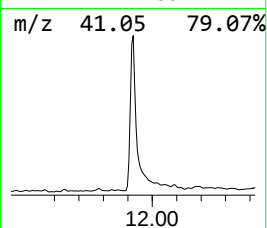
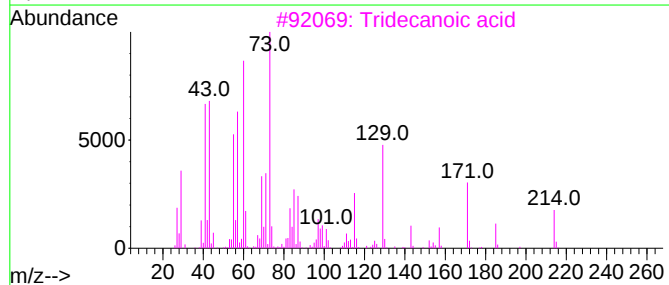
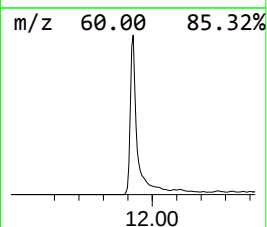
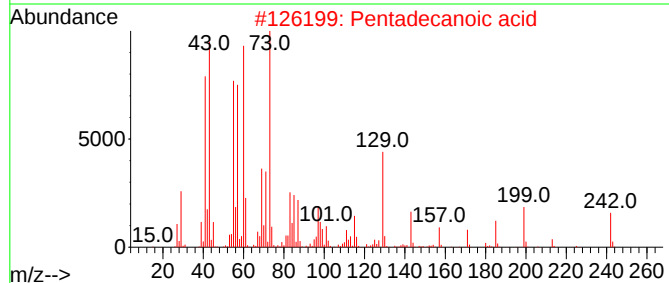
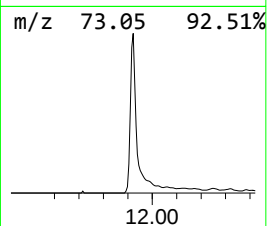
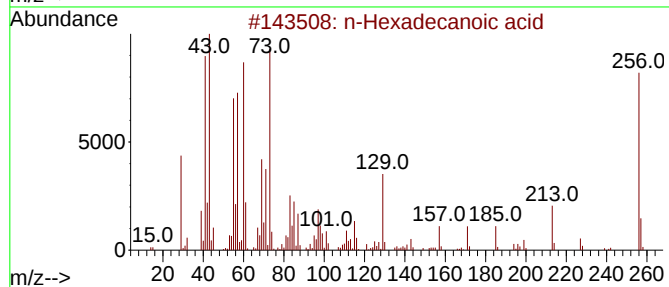
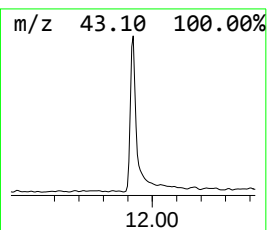
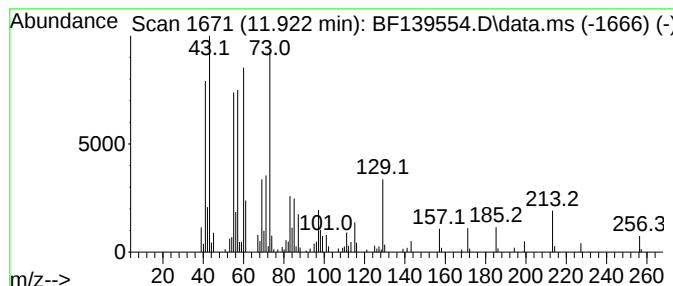
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	6.81 ng	215735	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Nonanoic acid	158	C9H18O2	000112-05-0	46



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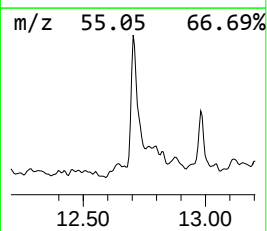
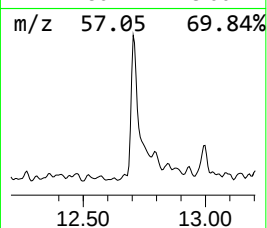
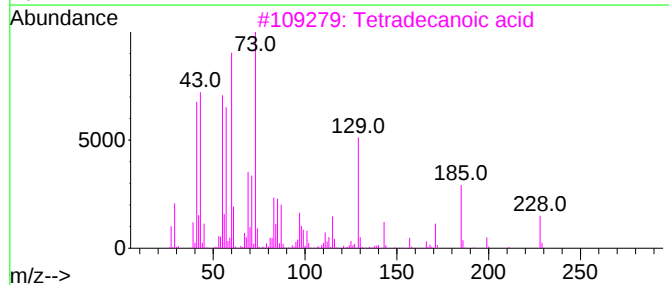
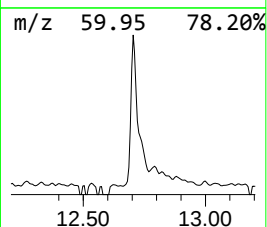
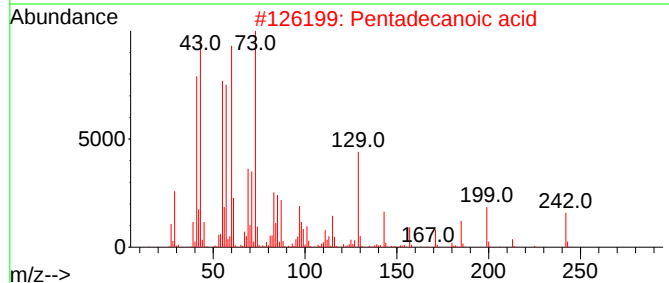
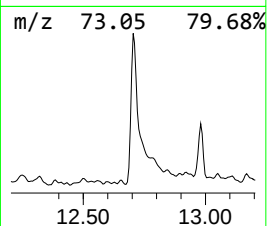
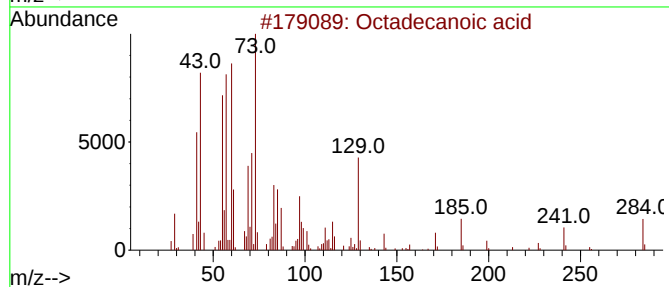
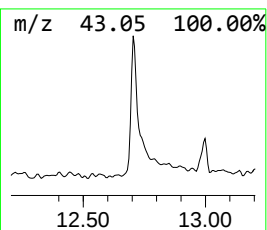
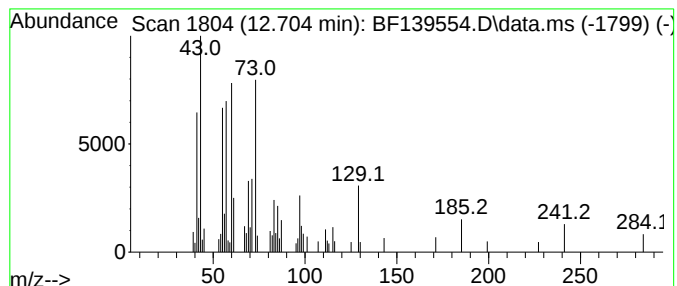
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	2.52 ng	79684	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



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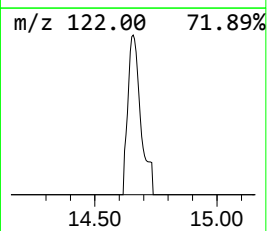
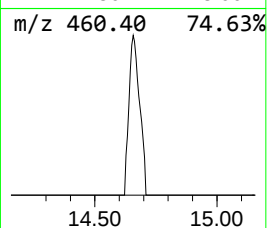
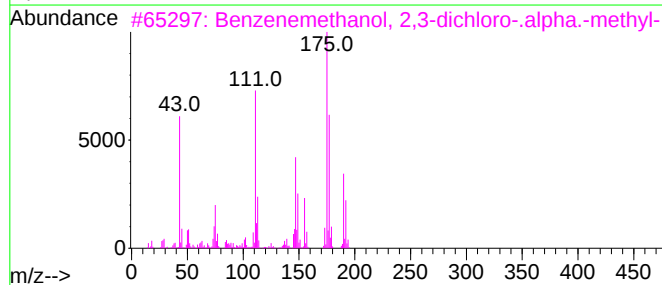
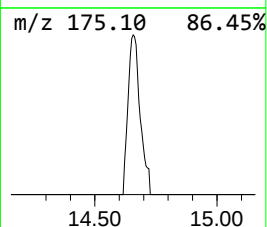
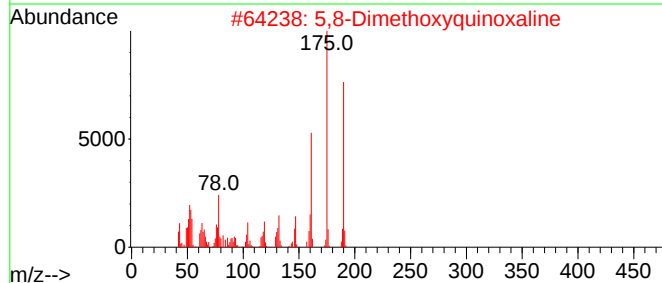
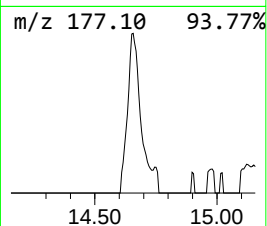
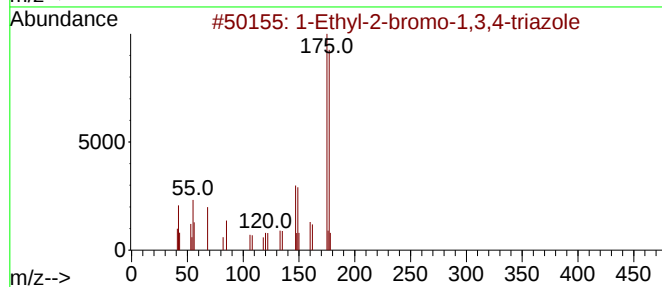
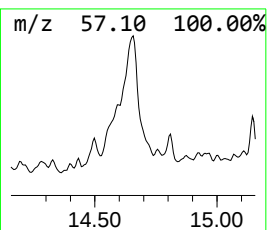
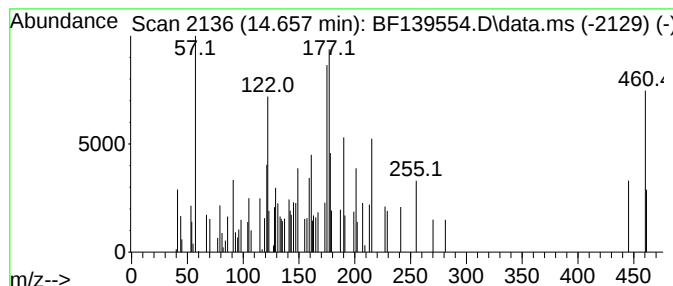
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown14.657 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	3.58 ng	70433	Chrysene-d12	14.033

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Ethyl-2-bromo-1,3,4-triazole	175	C4H6BrN3	064907-56-8	22
2		5,8-Dimethoxyquinoxaline	190	C10H10N2O2	019506-19-5	18
3		Benzenemethanol, 2,3-dichloro-.a...	190	C8H8Cl2O	054798-91-3	14
4		4-(2-Bromoethyl)-1,2,4-triazole	175	C4H6BrN3	1000459-77-6	12
5		Coumarin, 3,4-dihydro-4,5,7-trim...	190	C12H14O2	1000126-60-5	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139554.D
Acq On : 26 Sep 2024 18:59
Operator : RC/JU
Sample : P4176-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FB-1C-SYS2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.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
Butane, 2-metho...	2.157	176.6	ng	3889890	1	6.875	440464	20.0
2-Pentanone, 4-...	5.081	6.6	ng	145380	1	6.875	440464	20.0
Benzophenone	10.622	3.1	ng	96468	3	9.910	613849	20.0
n-Hexadecanoic ...	11.922	6.8	ng	215735	4	11.398	633435	20.0
Octadecanoic acid	12.704	2.5	ng	79684	4	11.398	633435	20.0
unknown14.657	14.657	3.6	ng	70433	5	14.033	392998	20.0