

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
 Data File : BF137345.D
 Acq On : 08 Feb 2024 18:49
 Operator : CG\JU
 Sample : P1368-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-306P-GW-20240201-0

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-BF013024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137345.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	13	16	20	rVB3	28489	39824	1.13%	0.214%
2	5.016	494	498	506	rVB	51316	60102	1.71%	0.323%
3	5.416	562	566	582	rBV	1619607	1507384	42.81%	8.098%
4	6.416	733	736	755	rBV	999716	925222	26.27%	4.970%
5	6.781	795	798	807	rBV	616657	594478	16.88%	3.194%
6	6.845	807	809	816	rVB	46698	45005	1.28%	0.242%
7	7.345	890	894	897	rBV	2000780	1972707	56.02%	10.598%
8	8.063	1012	1016	1034	rVB	876853	805967	22.89%	4.330%
9	8.380	1065	1070	1079	rBV2	41214	61093	1.73%	0.328%
10	9.145	1195	1200	1203	rBV	3877988	3521512	100.00%	18.918%
11	9.727	1294	1299	1303	rBV	151211	168826	4.79%	0.907%
12	9.816	1310	1314	1318	rBV	1018948	842751	23.93%	4.527%
13	9.922	1327	1332	1336	rBV2	308170	418464	11.88%	2.248%
14	10.610	1445	1449	1452	rBV	2220562	1981735	56.28%	10.646%
15	11.310	1564	1568	1576	rBV	882981	774452	21.99%	4.161%
16	11.716	1632	1637	1640	rBV	42444	44731	1.27%	0.240%
17	11.851	1656	1660	1665	rBV	231815	237660	6.75%	1.277%
18	12.427	1755	1758	1762	rVB	59901	47411	1.35%	0.255%
19	12.639	1791	1794	1799	rBV	78950	84133	2.39%	0.452%
20	12.757	1811	1814	1818	rVB	38923	37383	1.06%	0.201%
21	12.910	1835	1840	1843	rBV	3035011	2745456	77.96%	14.749%
22	13.821	1992	1995	2004	rVB	115966	122013	3.46%	0.655%
23	13.962	2015	2019	2029	rBV	596325	564619	16.03%	3.033%
24	14.462	2100	2104	2108	rBV2	57458	71377	2.03%	0.383%
25	14.857	2166	2171	2176	rBV2	57717	84876	2.41%	0.456%
26	15.298	2242	2246	2254	rVB2	57031	84605	2.40%	0.455%
27	15.445	2266	2271	2277	rBV	496037	618886	17.57%	3.325%
28	15.821	2329	2335	2343	rVB3	45228	92488	2.63%	0.497%
29	16.439	2435	2440	2448	rBV4	28948	59200	1.68%	0.318%

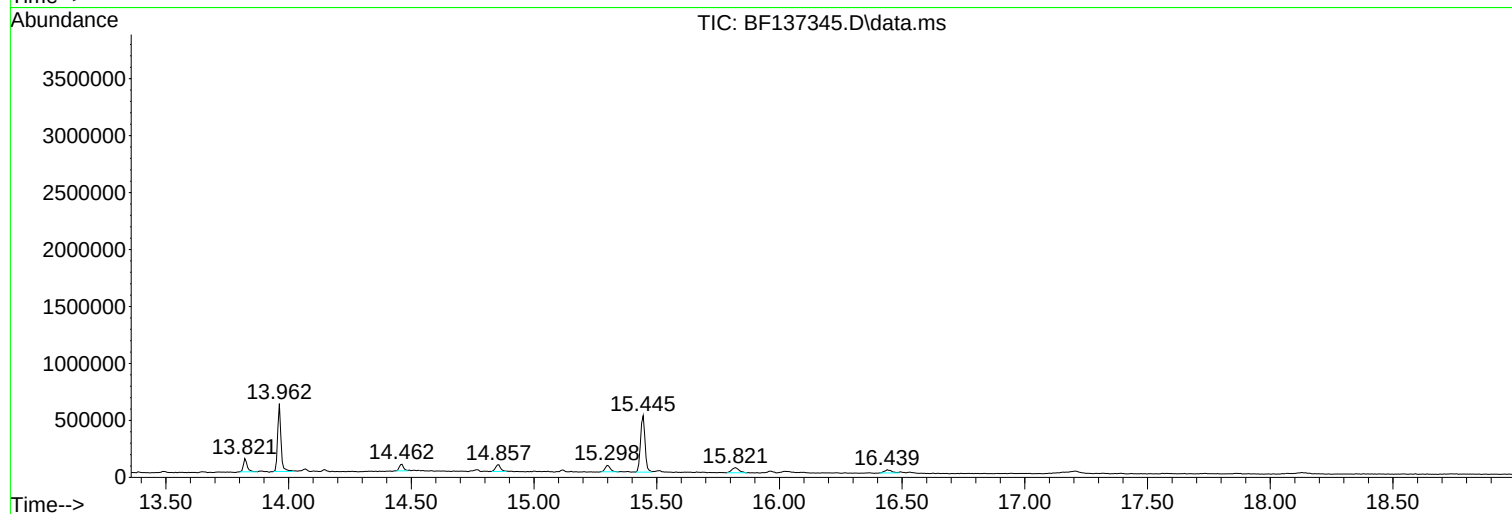
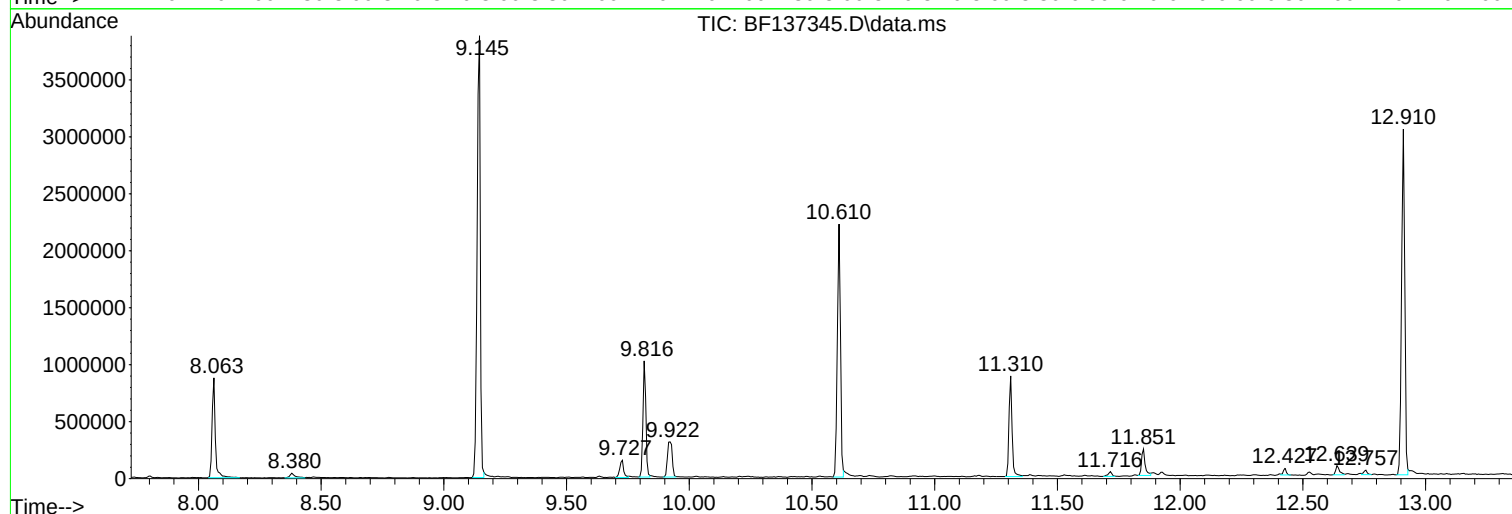
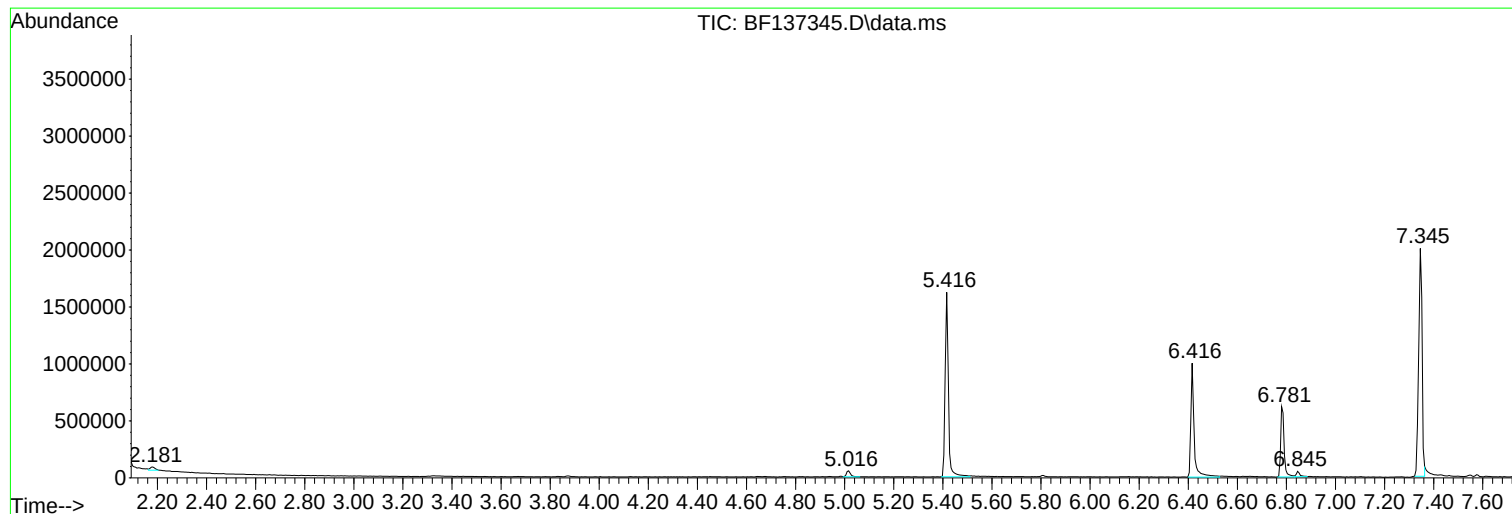
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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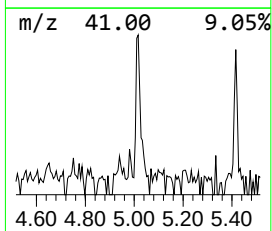
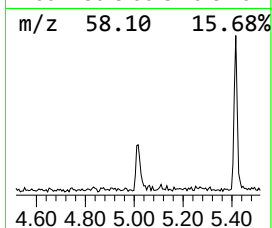
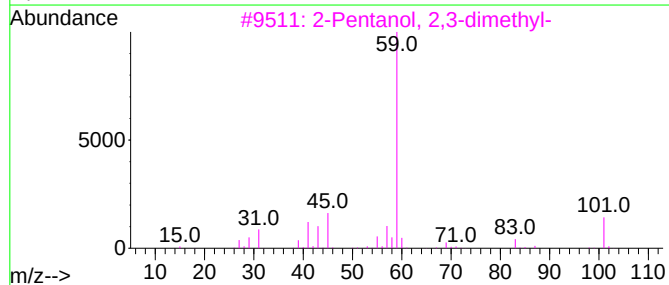
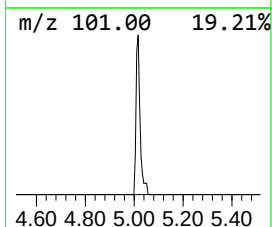
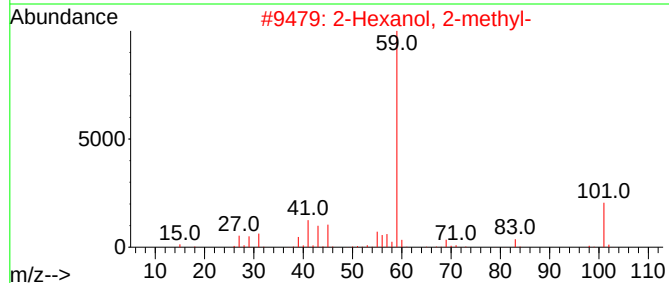
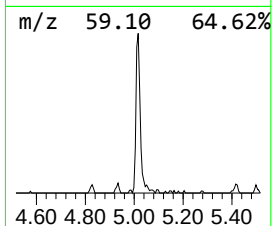
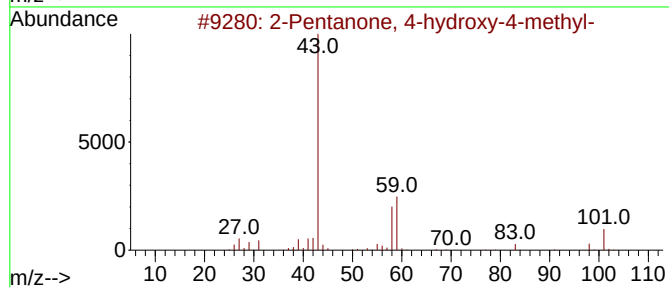
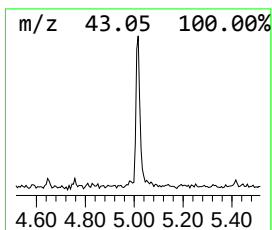
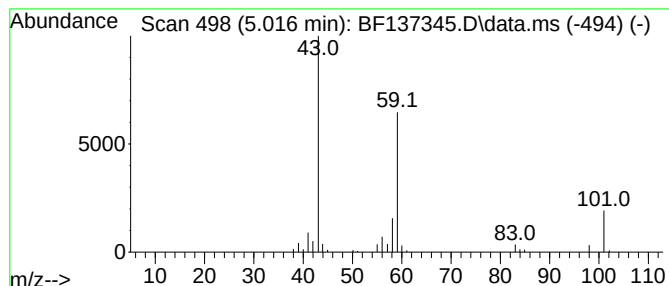
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	2.02 ng	60102	1,4-Dichlorobenzene-d4	6.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
3	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	1,2-Butanediol	90	C4H10O2	000584-03-2	25		



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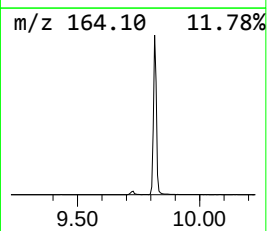
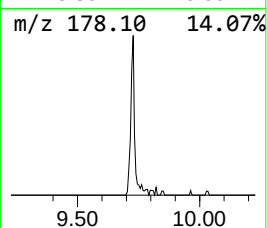
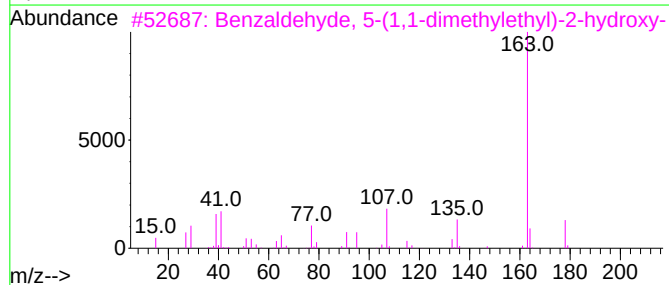
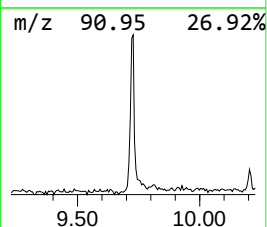
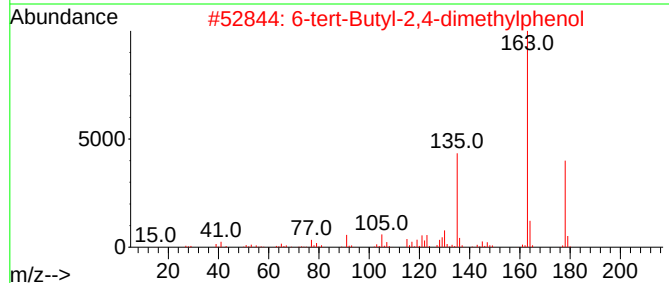
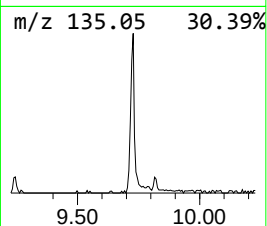
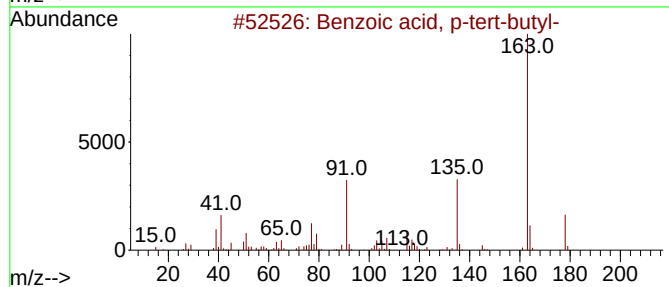
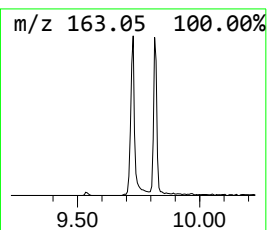
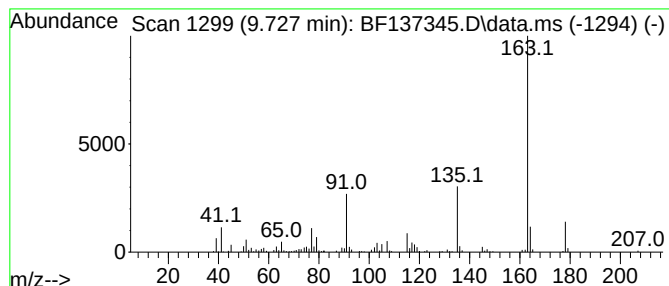
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzoic acid, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.727	4.01 ng	168826	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	93
2			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	74
3			Benzaldehyde, 5-(1,1-dimethylethyl)-2-hydroxy-	178	C11H14O2	002725-53-3	72
4			Benzoic acid, 4-acetyl-, methyl ester	178	C10H10O3	003609-53-8	64
5			1,3-Benzenedicarboxylic acid, diethyl ester	194	C10H10O4	001459-93-4	64



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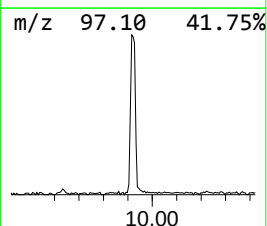
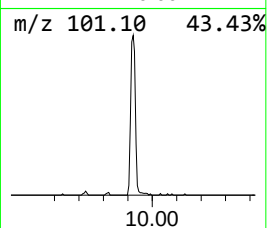
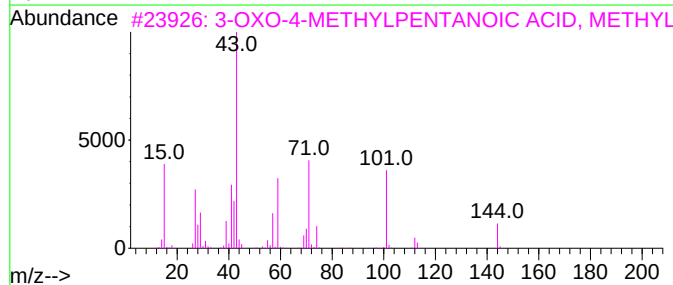
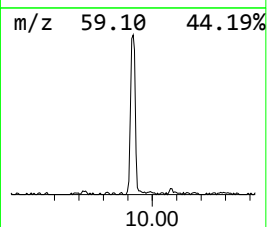
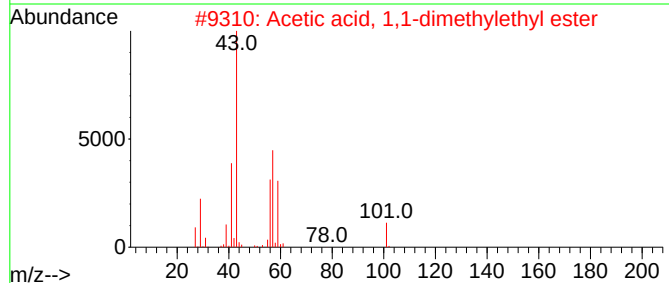
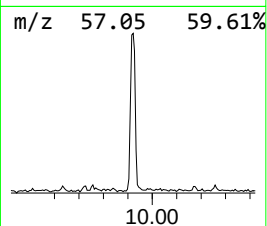
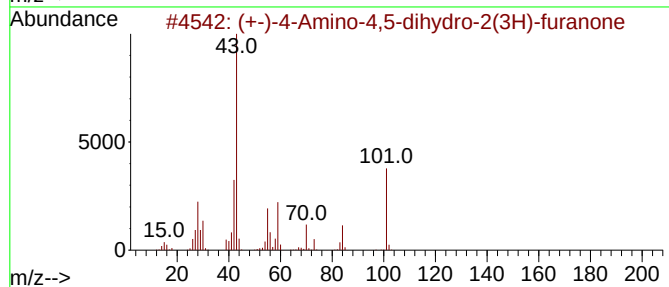
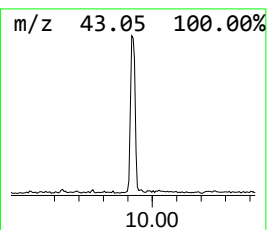
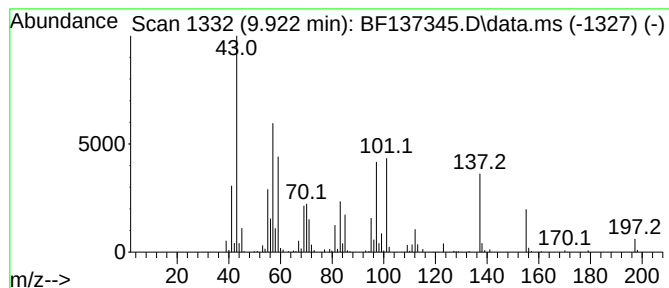
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown9.922 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.922	9.93 ng	418464	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	22		
3	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	16		
4	2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1010191-06-9	14		
5	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	12		



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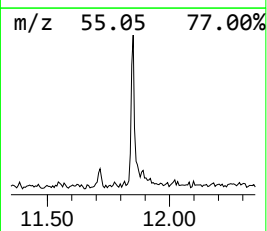
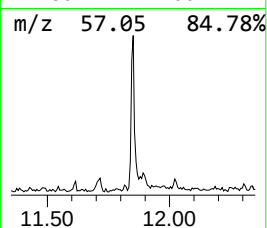
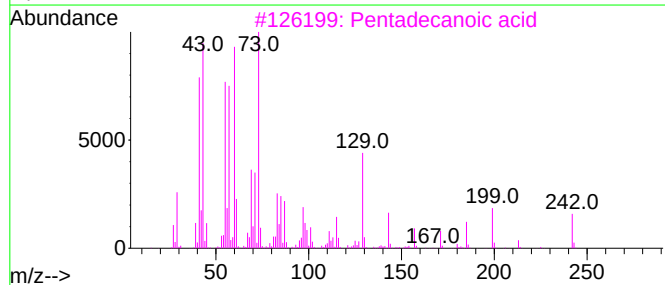
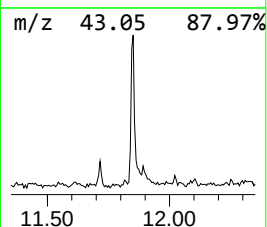
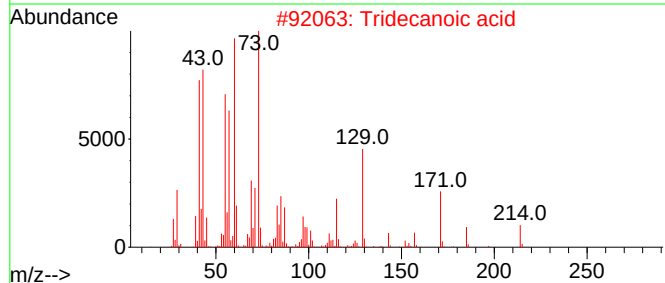
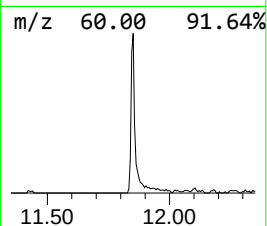
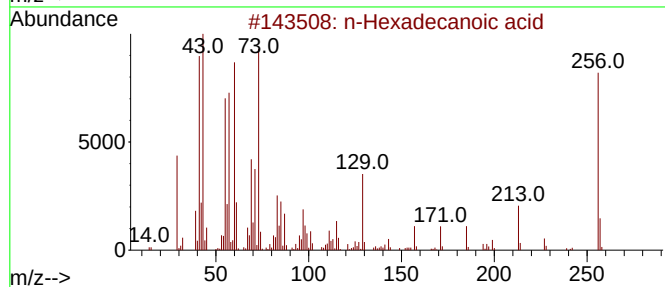
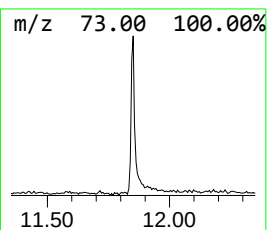
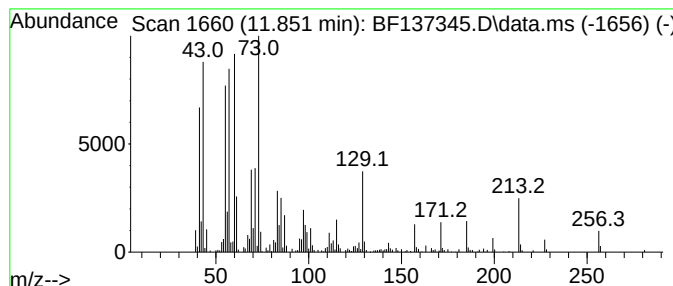
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	6.14 ng	237660	Phenanthrene-d10	11.310

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53



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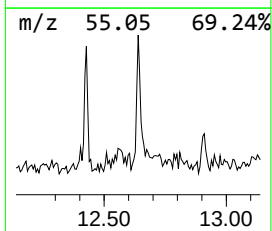
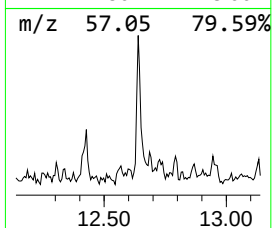
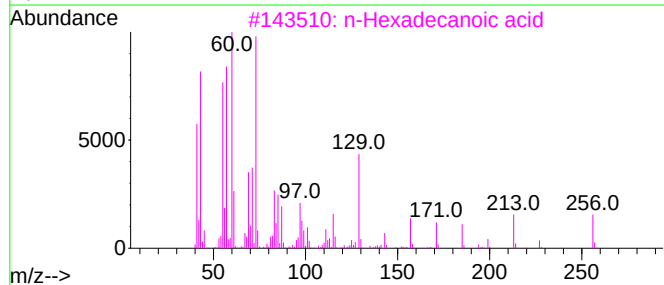
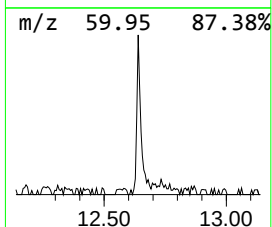
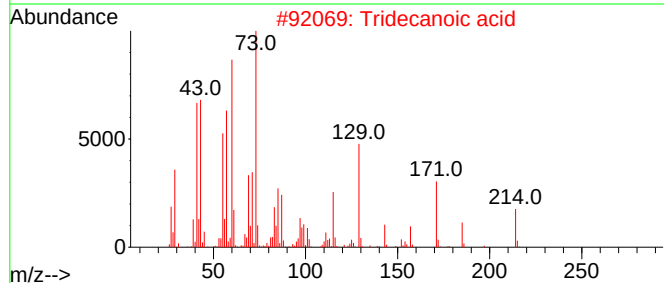
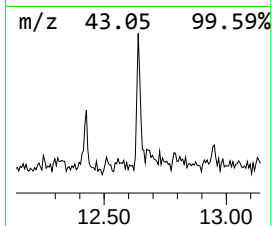
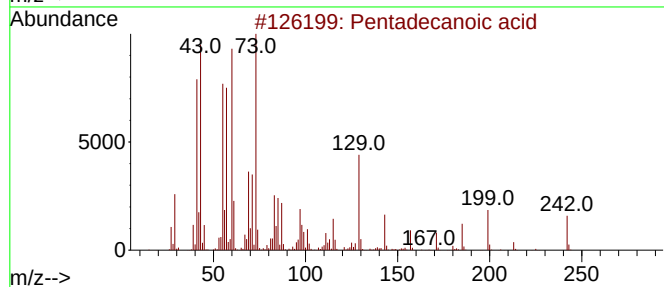
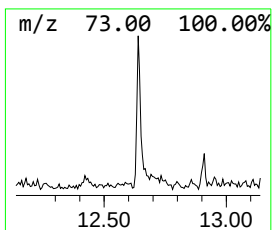
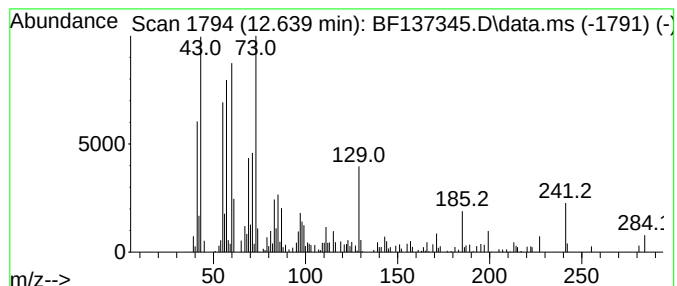
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Peak Number 5 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	2.98 ng	84133	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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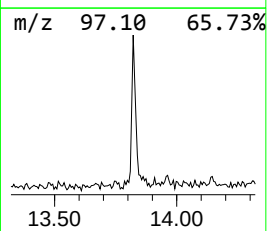
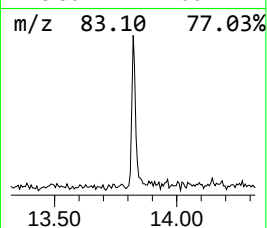
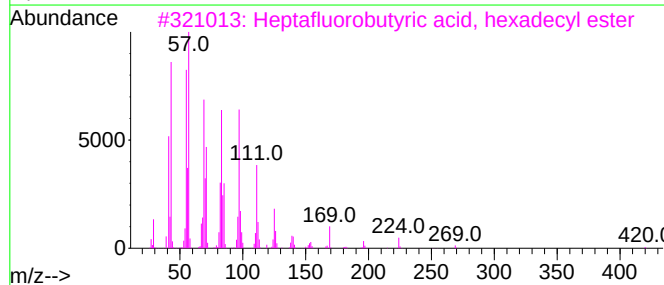
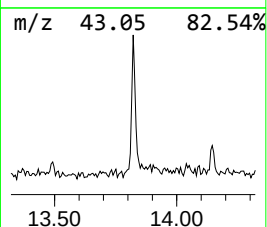
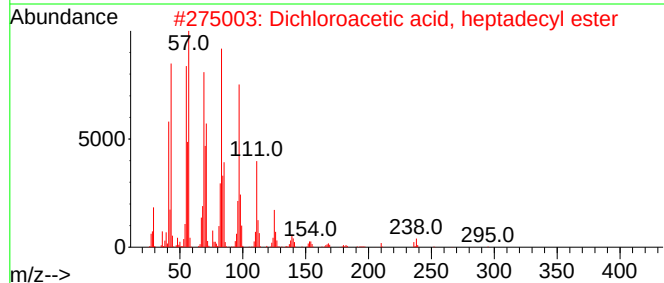
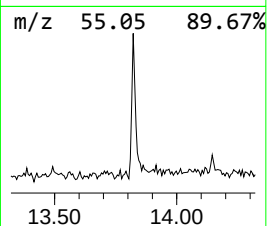
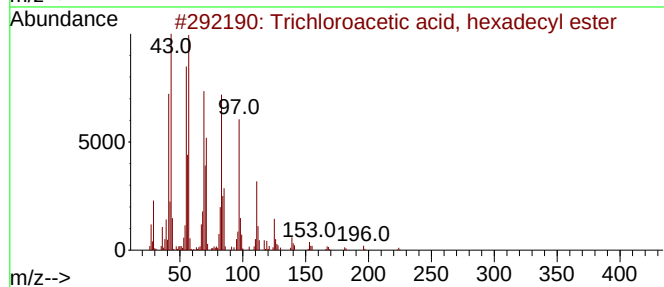
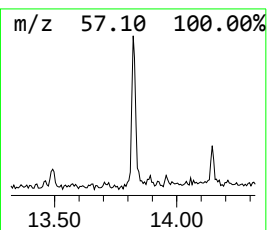
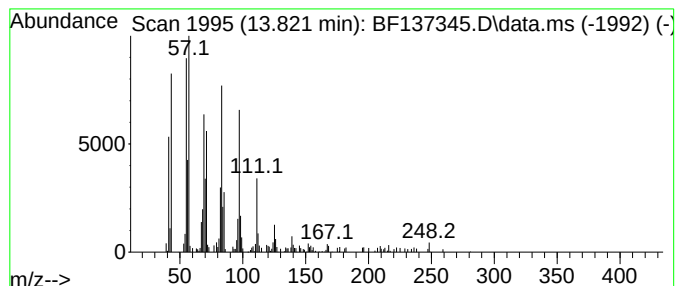
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	4.32 ng	122013	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4			1-Hexacosene	364	C26H52	018835-33-1	91
5			17-Pentatriacontene	491	C35H70	006971-40-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137345.D
Acq On : 08 Feb 2024 18:49
Operator : CG\JU
Sample : P1368-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-306P-GW-20240201-0

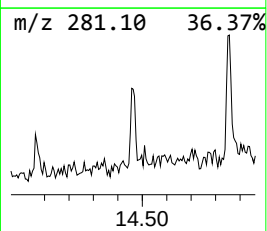
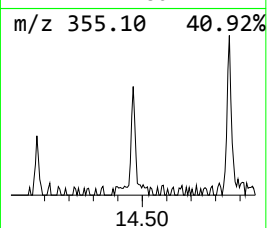
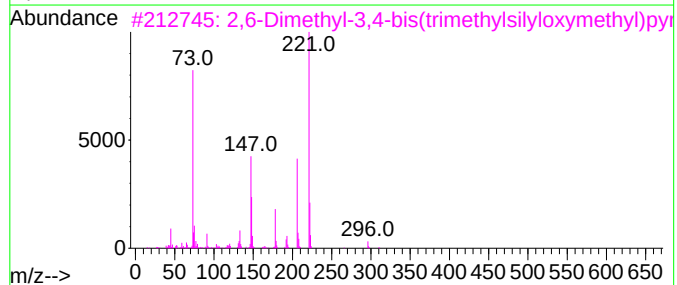
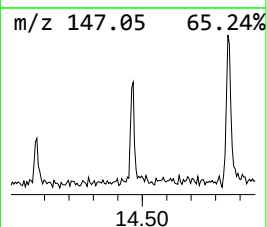
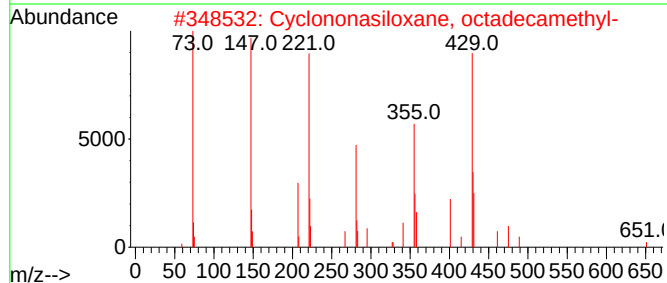
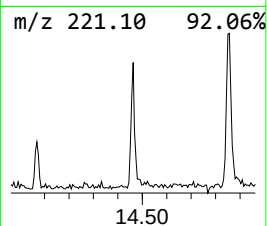
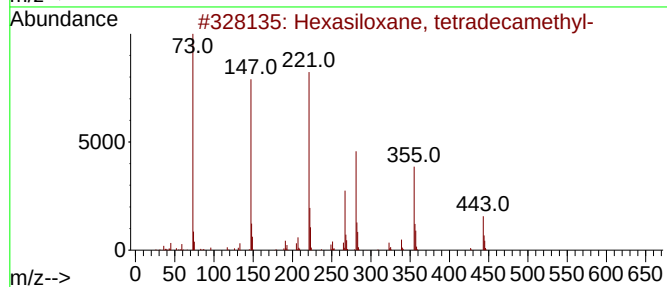
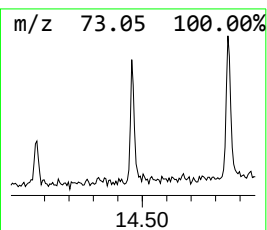
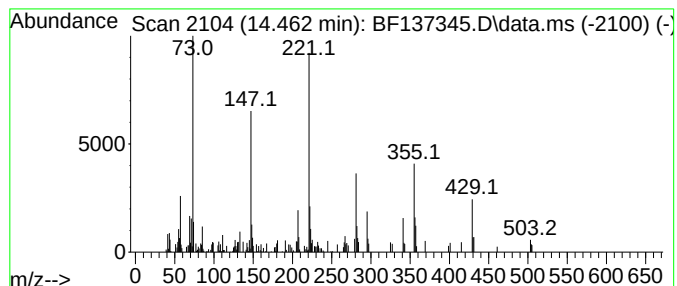
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexasiloxane, tetradecamethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.463	2.53 ng	71377	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	80
2			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
3			2,6-Dimethyl-3,4-bis(trimethylsi...	311	C15H29NO2Si2	1000079-52-1	43
4			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	38
5			2-Amino-2-oxo-acetic acid, N-[3,...	221	C12H15NO3	024451-17-0	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020824\
Data File : BF137345.D
Acq On : 08 Feb 2024 18:49
Operator : CG\JU
Sample : P1368-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MR-306P-GW-20240201-0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.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-...	5.016	2.0	ng	60102	1	6.786	594478	20.0
Benzoic acid, p...	9.727	4.0	ng	168826	3	9.816	842751	20.0
unknown9.922	9.922	9.9	ng	418464	3	9.816	842751	20.0
n-Hexadecanoic ...	11.851	6.1	ng	237660	4	11.310	774452	20.0
Pentadecanoic acid	12.639	3.0	ng	84133	5	13.963	564619	20.0
Trichloroacetic...	13.821	4.3	ng	122013	5	13.963	564619	20.0
Hexasiloxane, t...	14.463	2.5	ng	71377	5	13.963	564619	20.0