

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
 Data File : BF140268.D
 Acq On : 07 Nov 2024 12:14
 Operator : RC/JU
 Sample : P4701-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BP-F4

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-BF110524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140268.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	8	17	30	rVB	863186	1467579	33.19%	5.047%
2	2.299	30	35	43	rVB	30446	52968	1.20%	0.182%
3	5.104	504	512	523	rVB	120646	210876	4.77%	0.725%
4	5.498	572	579	584	rBV	2552469	3454505	78.12%	11.880%
5	6.498	742	749	754	rBV	2514958	3567045	80.67%	12.267%
6	6.875	808	813	818	rBV	589788	714620	16.16%	2.458%
7	7.434	901	908	913	rBV	1755245	2363637	53.45%	8.128%
8	8.157	1025	1031	1038	rBV	699566	927863	20.98%	3.191%
9	9.234	1207	1214	1219	rBV	3217708	4320025	97.69%	14.856%
10	9.910	1324	1329	1345	rVB	826513	1098522	24.84%	3.778%
11	10.628	1446	1451	1458	rBV	209958	256874	5.81%	0.883%
12	10.704	1458	1464	1479	rBV	2202490	2878645	65.10%	9.899%
13	11.404	1578	1583	1590	rBV	899120	1130130	25.56%	3.886%
14	11.928	1664	1672	1686	rBV	185103	321478	7.27%	1.106%
15	12.992	1847	1853	1858	rBV	3397126	4422015	100.00%	15.207%
16	13.904	2003	2008	2024	rBV2	76035	214893	4.86%	0.739%
17	14.057	2028	2034	2045	rVB	596720	797672	18.04%	2.743%
18	14.845	2163	2168	2180	rBV2	77351	152634	3.45%	0.525%
19	15.568	2285	2291	2303	rBV	446531	726922	16.44%	2.500%

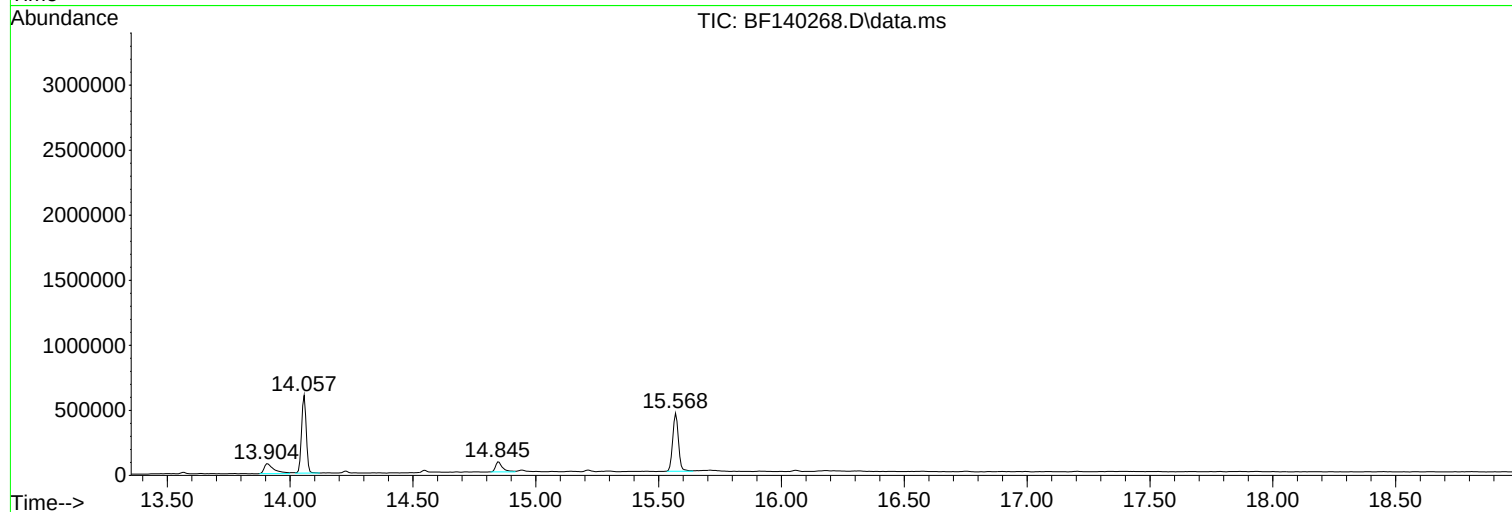
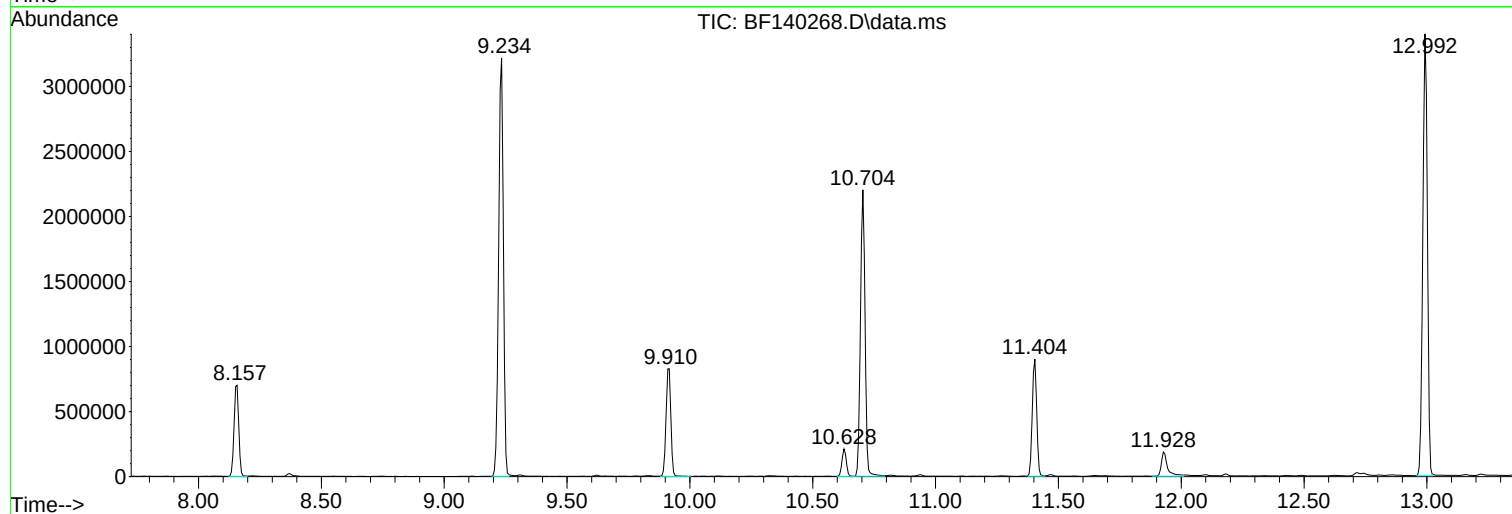
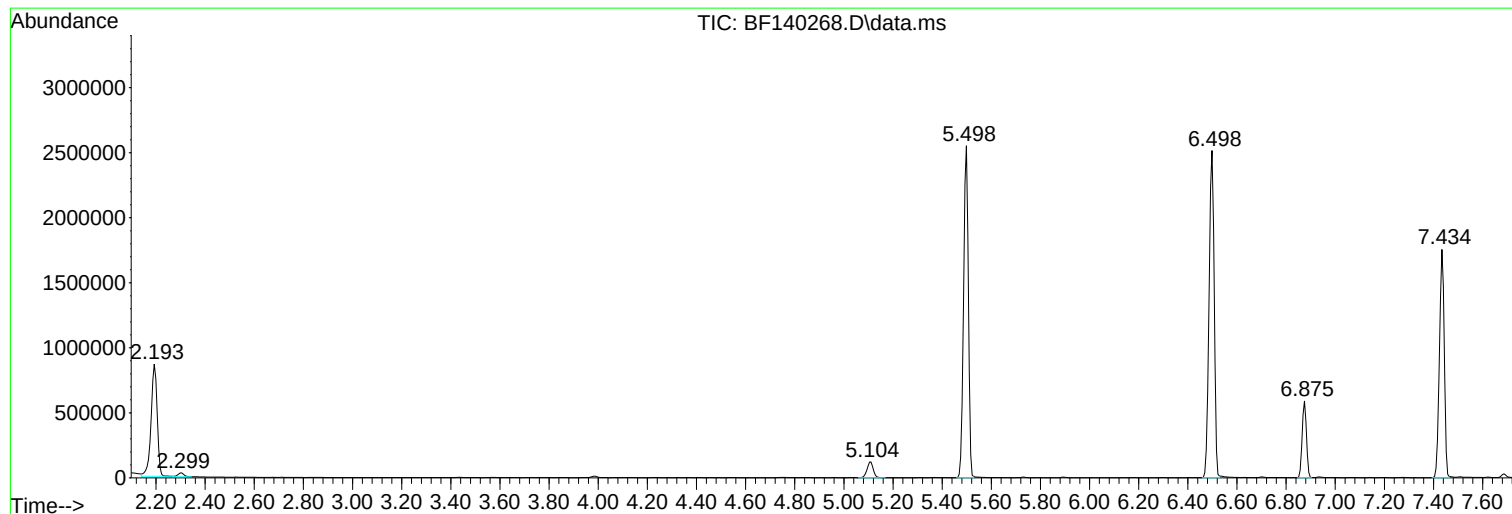
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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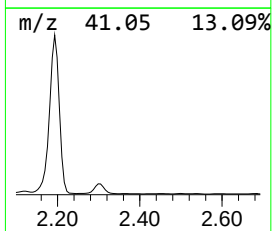
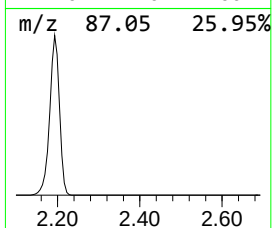
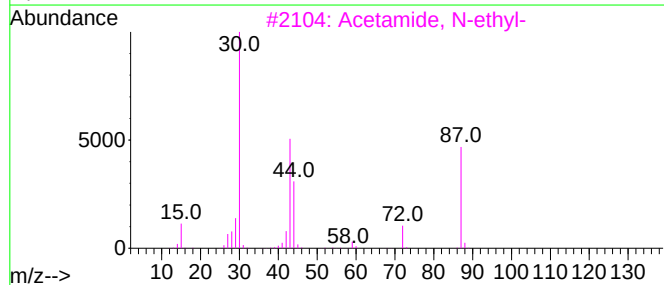
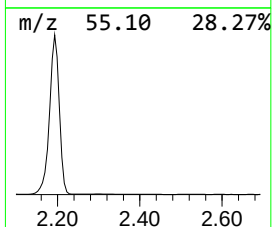
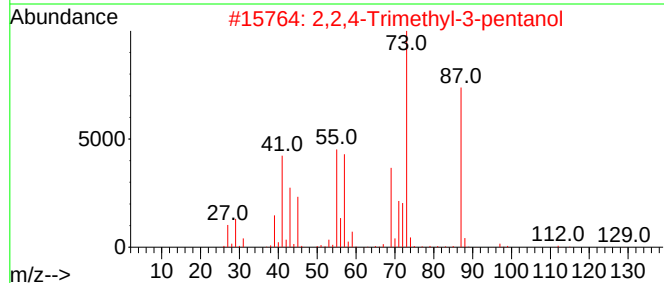
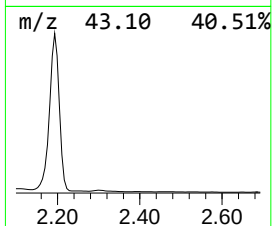
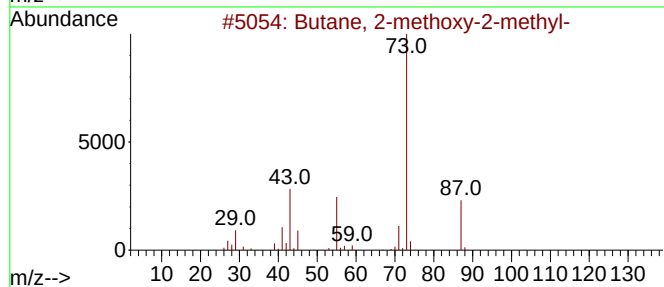
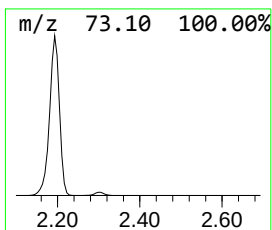
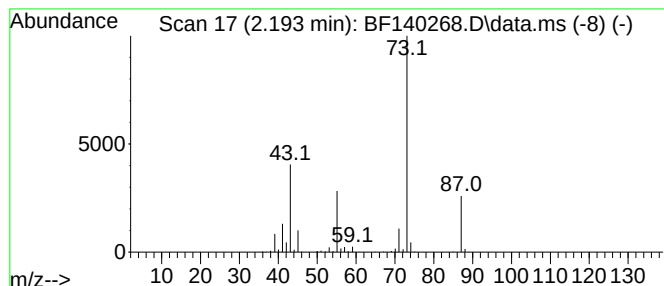
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	41.07 ng	1467580	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	39
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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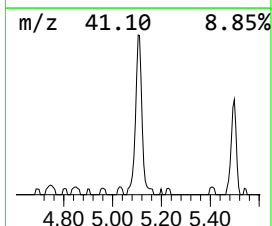
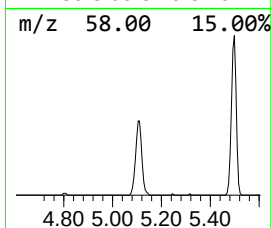
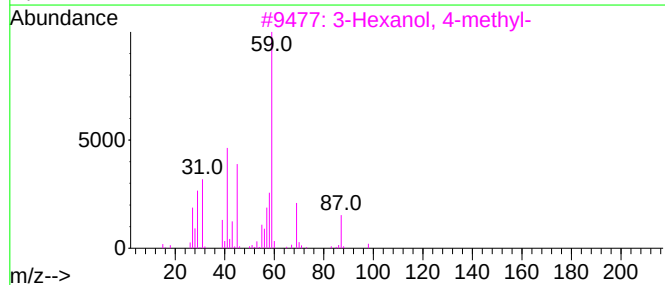
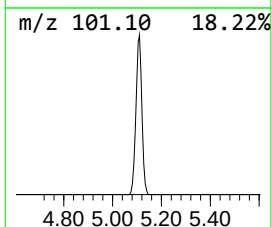
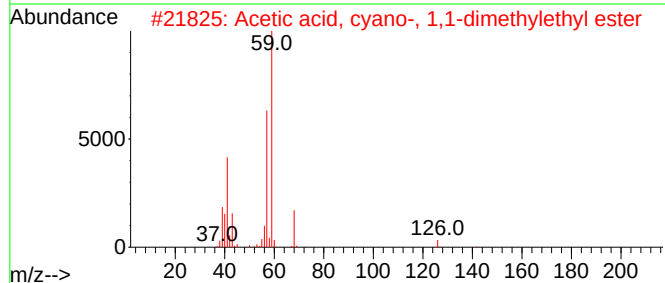
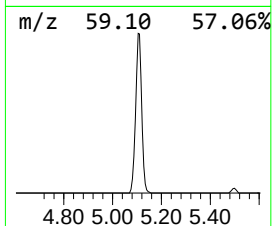
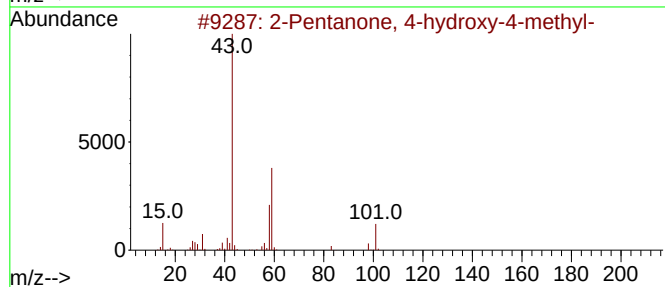
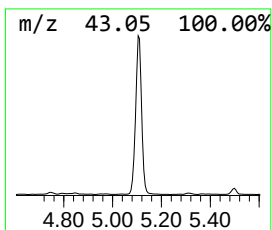
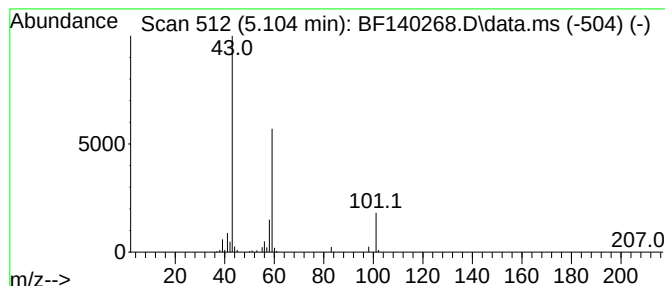
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	5.90 ng	210876	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	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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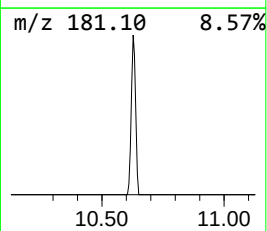
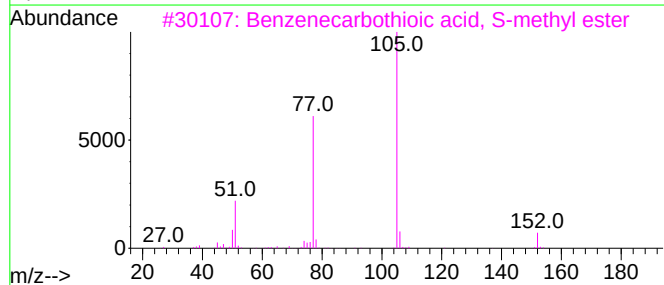
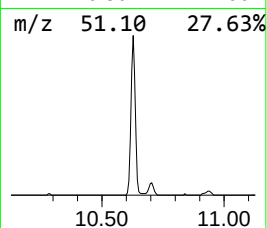
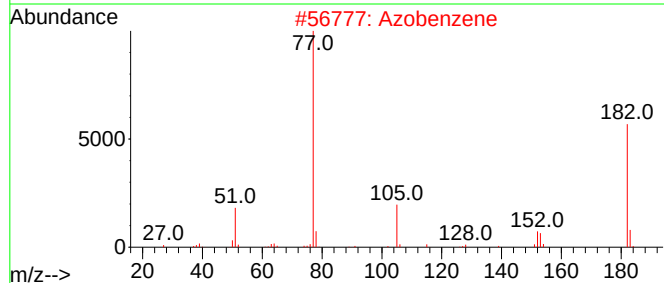
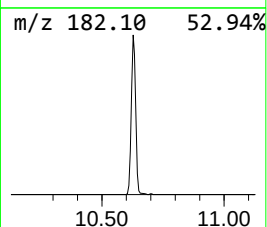
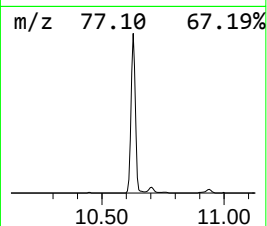
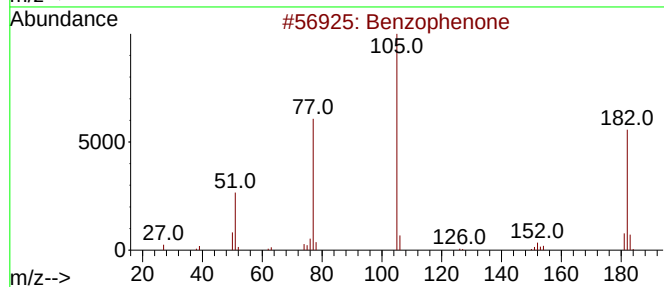
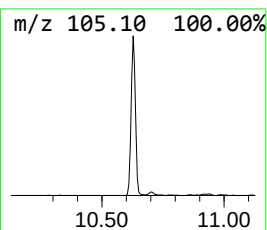
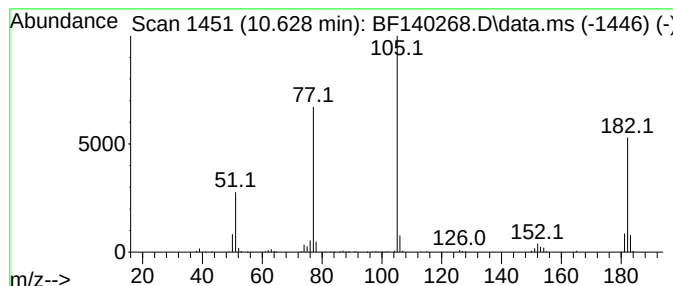
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Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	4.68 ng	256874	Acenaphthene-d10	9.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47



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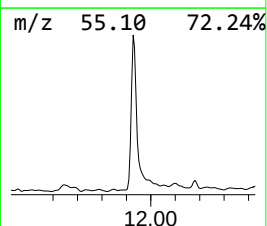
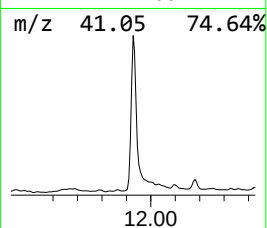
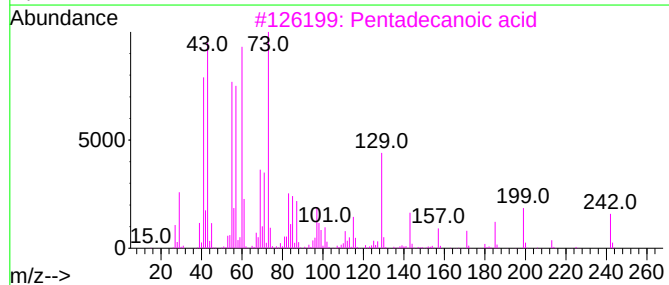
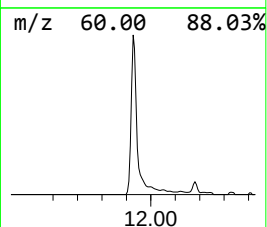
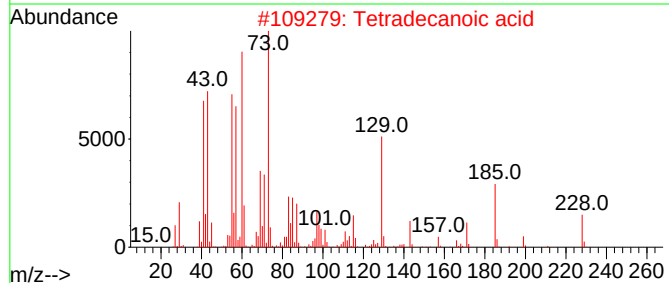
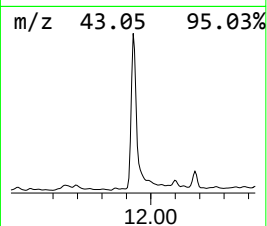
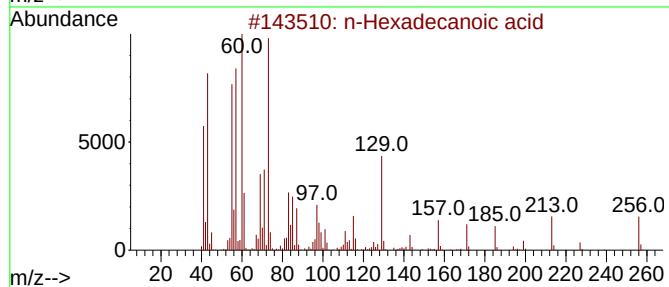
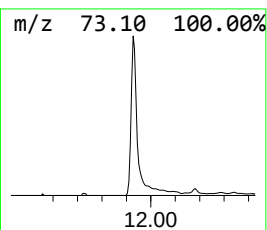
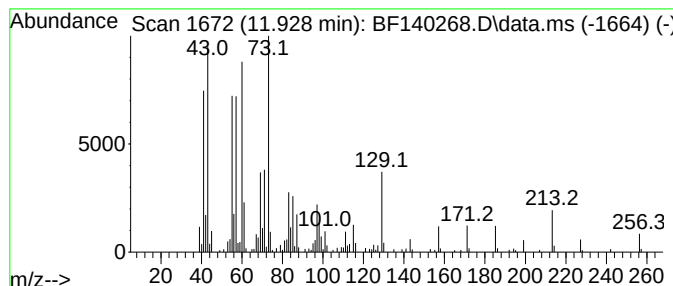
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	5.69 ng	321478	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	81
5			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20



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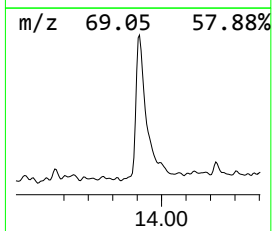
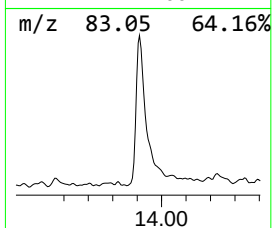
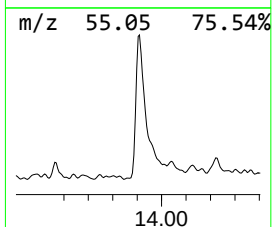
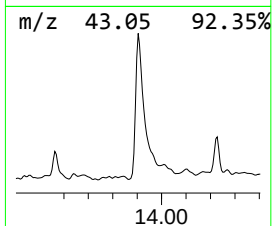
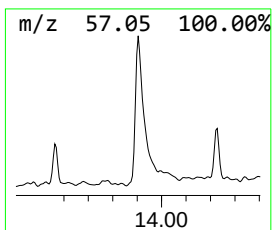
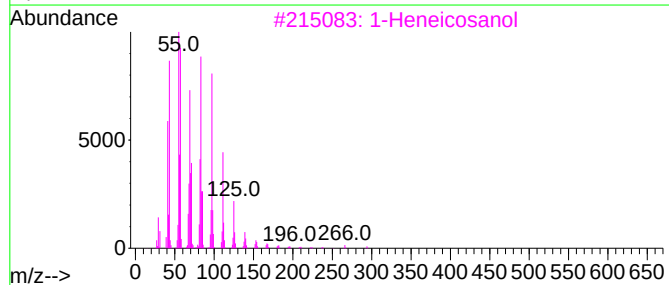
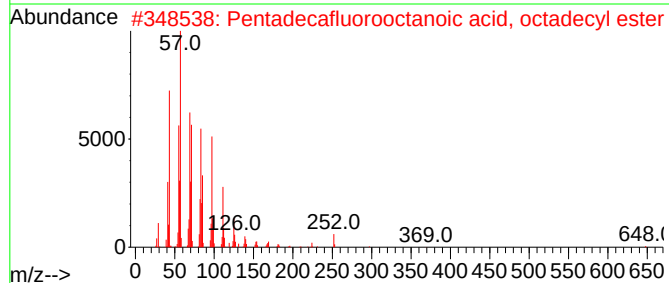
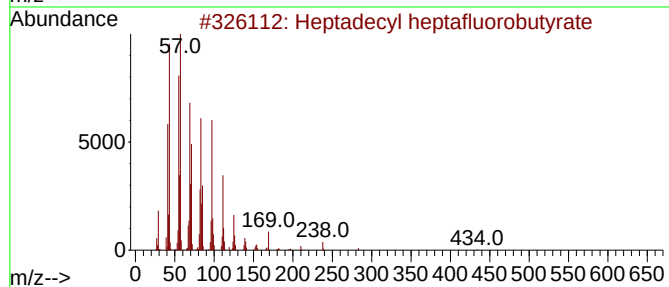
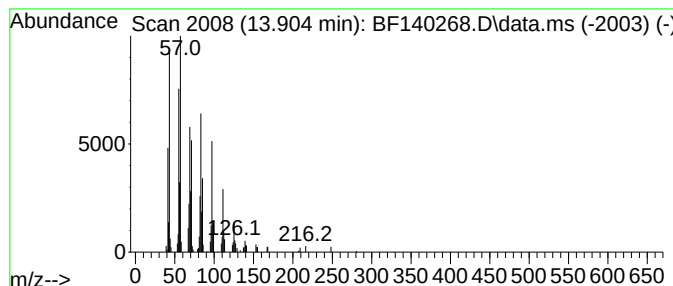
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	5.39 ng	214893	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			1-Hexacosene	364	C26H52	018835-33-1	91
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



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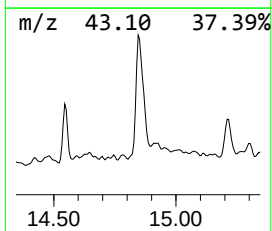
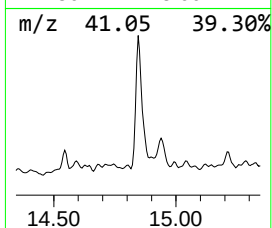
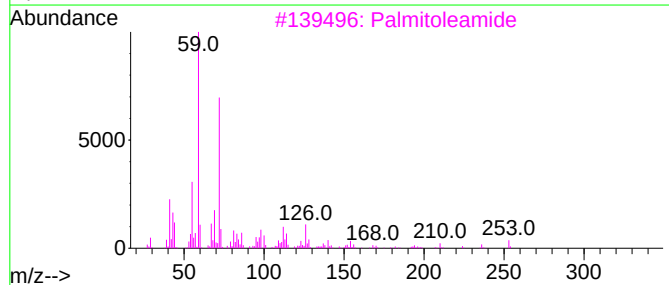
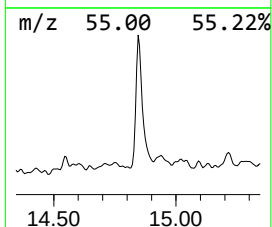
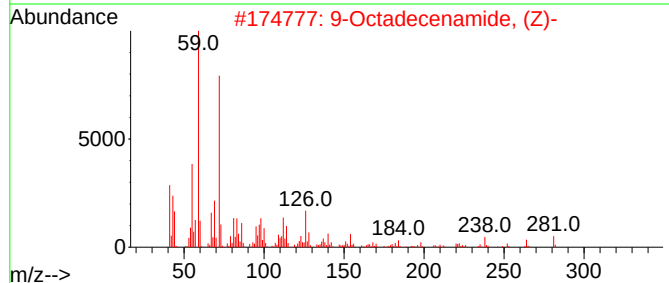
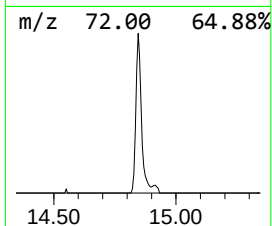
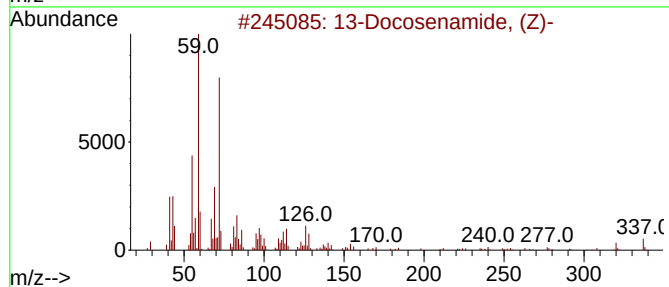
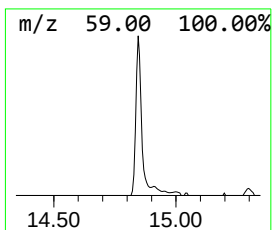
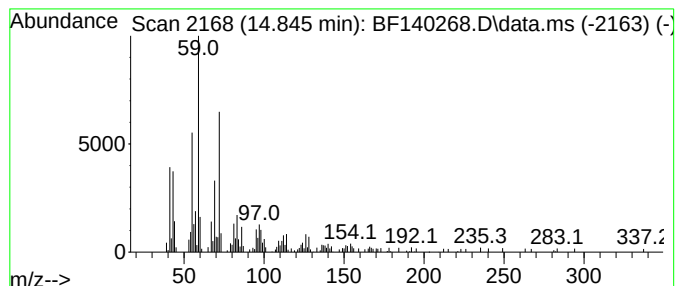
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.845	4.20 ng	152634	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
3			Palmitoleamide	253	C16H31NO	106010-22-4	72
4			Hexadecanamide	255	C16H33NO	000629-54-9	72
5			9-Octadecenamide	281	C18H35NO	003322-62-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140268.D
Acq On : 07 Nov 2024 12:14
Operator : RC/JU
Sample : P4701-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BP-F4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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
Butane, 2-metho...	2.193	41.1	ng	1467580	1	6.875	714620	20.0
2-Pentanone, 4-...	5.104	5.9	ng	210876	1	6.875	714620	20.0
Benzophenone	10.628	4.7	ng	256874	3	9.916	1098520	20.0
n-Hexadecanoic ...	11.928	5.7	ng	321478	4	11.404	1130130	20.0
Heptadecyl hept...	13.904	5.4	ng	214893	5	14.057	797672	20.0
13-Docosenamide...	14.845	4.2	ng	152634	6	15.568	726922	20.0