

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
 Data File : BF138160.D
 Acq On : 07 Jun 2024 15:05
 Operator : CG\JU
 Sample : P2704-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WCS-TPO

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-BF060524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	16	24	29	rBV	4804474	6068603	63.62%	9.224%
2	3.434	225	229	252	rBV	133616	288451	3.02%	0.438%
3	5.528	579	585	588	rBV	7489504	7360813	77.16%	11.188%
4	6.528	749	755	758	rBV	6697604	7662674	80.33%	11.647%
5	6.904	816	819	822	rBV	2729673	2007506	21.04%	3.051%
6	7.469	909	915	918	rBV	5212444	4901304	51.38%	7.449%
7	7.716	954	957	960	rBV	266021	192806	2.02%	0.293%
8	8.086	1016	1020	1028	rBV	118968	136407	1.43%	0.207%
9	8.186	1033	1037	1040	rBV	3435186	2686797	28.17%	4.084%
10	8.492	1086	1089	1098	rBV	321144	305745	3.21%	0.465%
11	9.263	1215	1220	1223	rBV	10942219	9539486	100.00%	14.499%
12	9.939	1331	1335	1338	rBV	4062747	3154234	33.07%	4.794%
13	10.033	1345	1351	1360	rBV2	171407	236226	2.48%	0.359%
14	10.727	1464	1469	1472	rBV	6714606	5754159	60.32%	8.746%
15	11.422	1584	1587	1591	rBV	3237834	2939780	30.82%	4.468%
16	11.951	1673	1677	1682	rBV	555127	523811	5.49%	0.796%
17	12.733	1807	1810	1815	rBV	147738	160671	1.68%	0.244%
18	13.010	1853	1857	1861	rBV	7733172	7440813	78.00%	11.309%
19	13.492	1934	1939	1949	rBV	1014911	1056887	11.08%	1.606%
20	13.927	2008	2013	2024	rBV3	159562	400168	4.19%	0.608%
21	14.063	2032	2036	2045	rBV	1701765	1504710	15.77%	2.287%
22	15.545	2282	2288	2294	rBV	984020	1305286	13.68%	1.984%
23	17.021	2533	2539	2553	rVB3	53464	166436	1.74%	0.253%

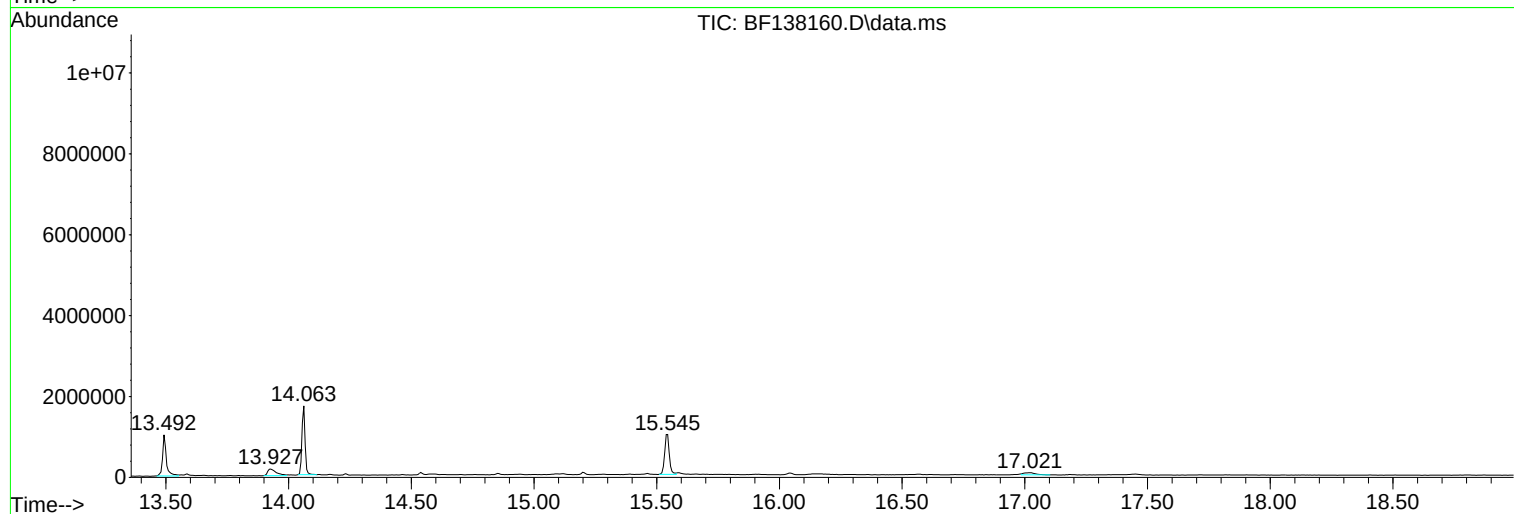
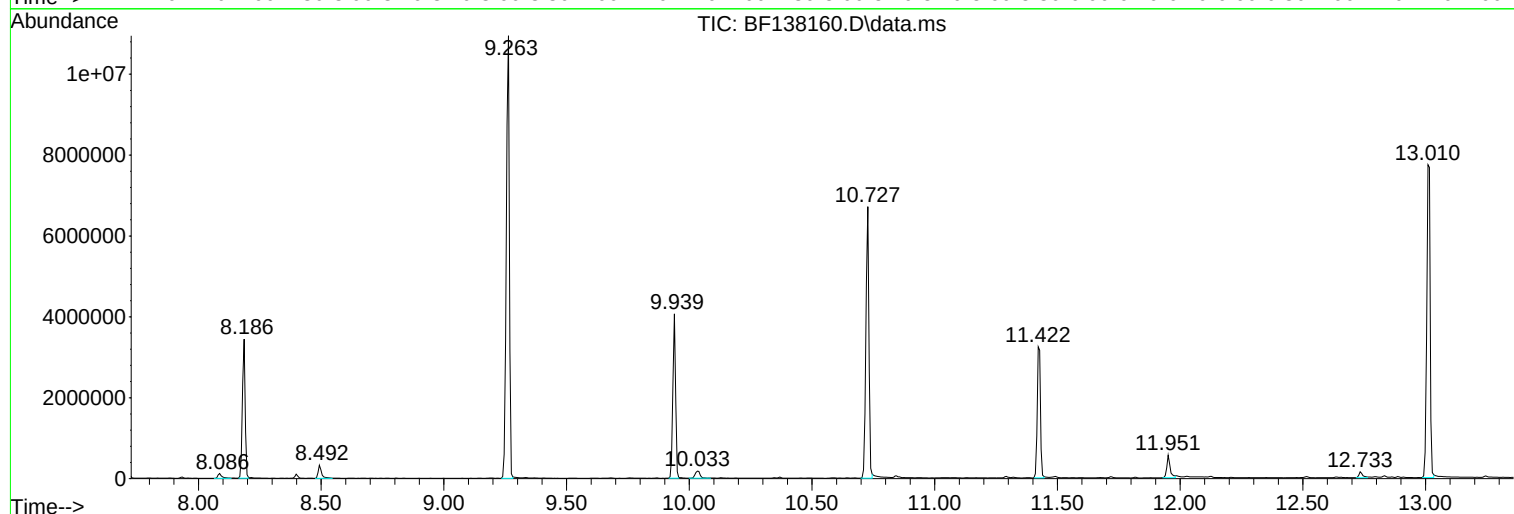
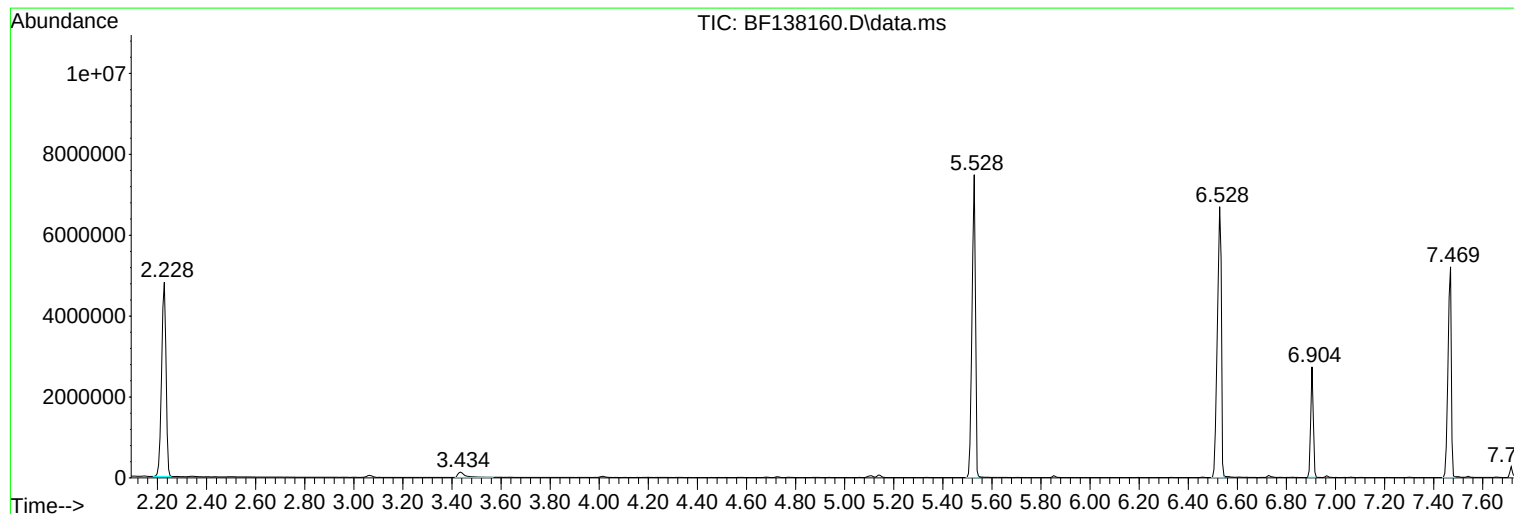
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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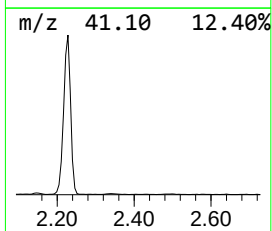
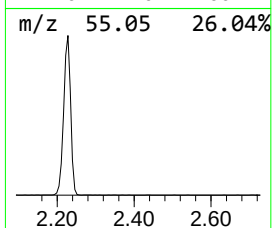
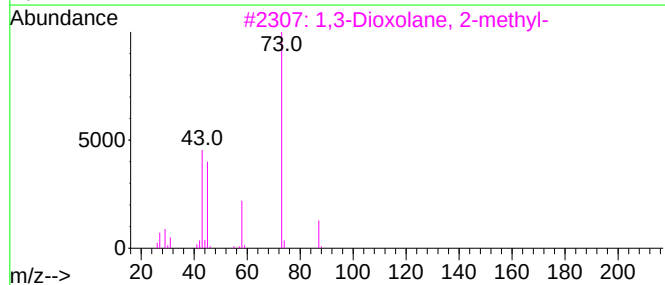
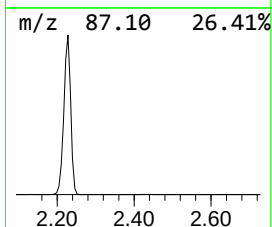
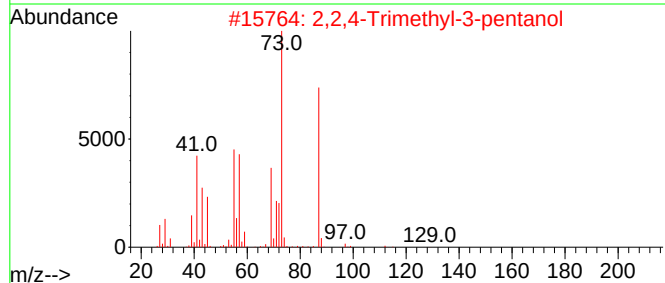
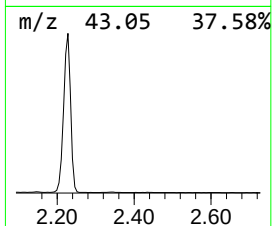
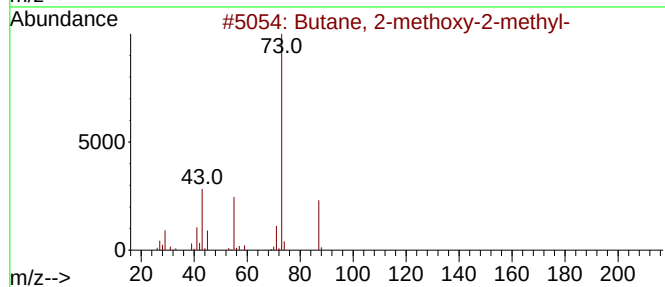
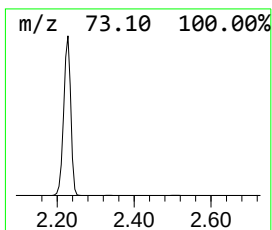
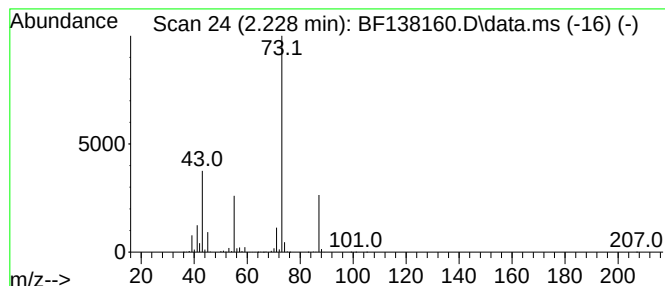
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	60.46 ng	6068600	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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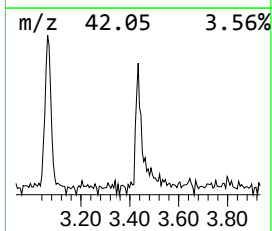
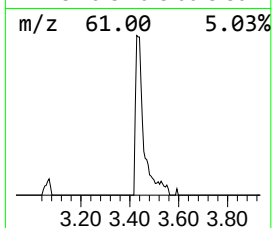
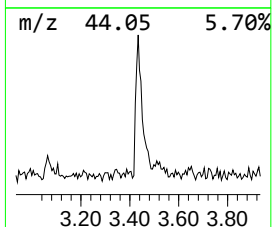
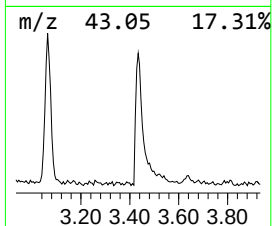
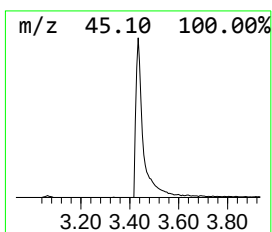
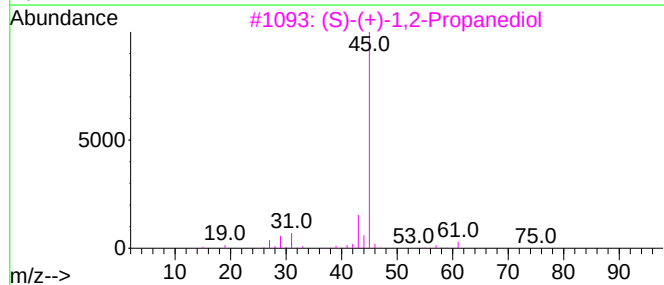
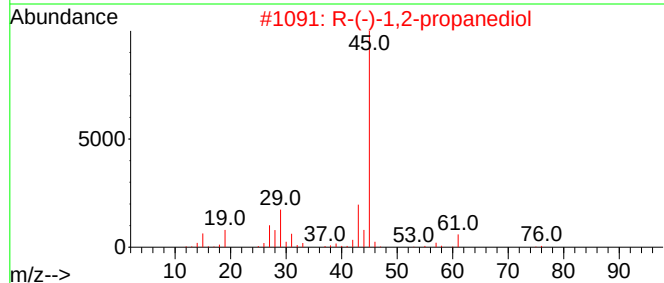
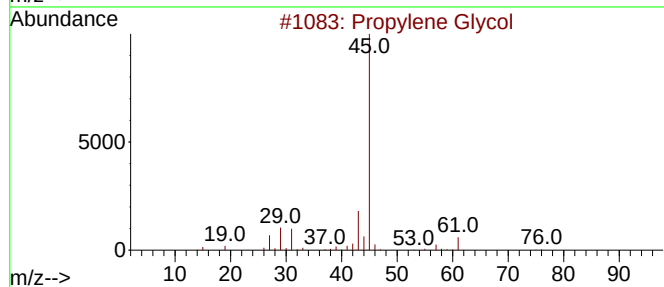
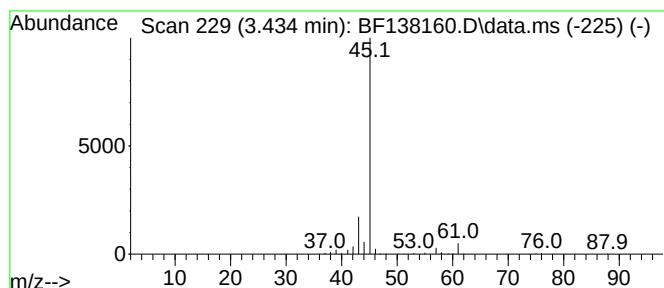
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.434	2.87 ng	288451	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			2-Pentanol	88	C5H12O	006032-29-7	9



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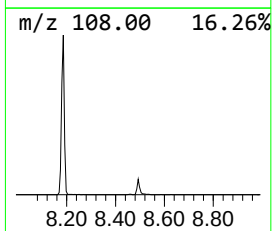
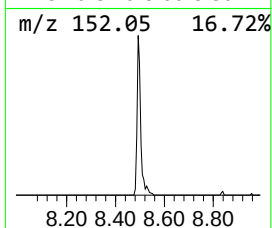
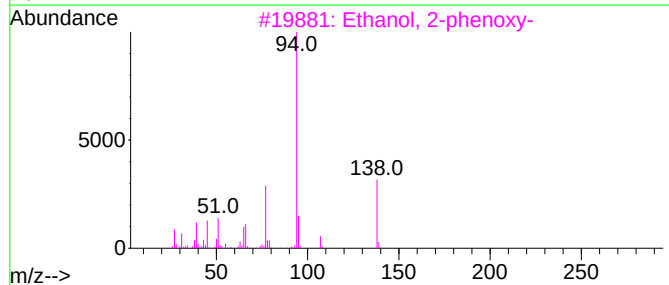
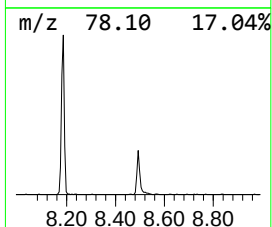
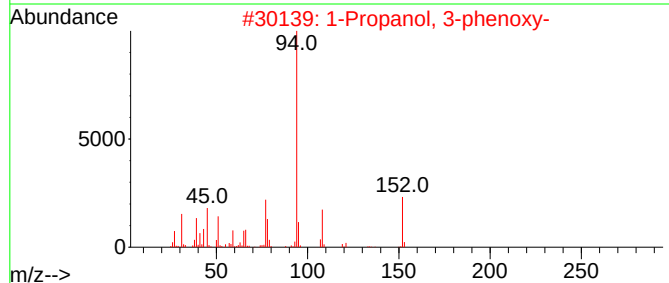
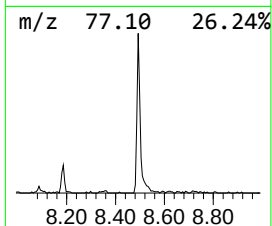
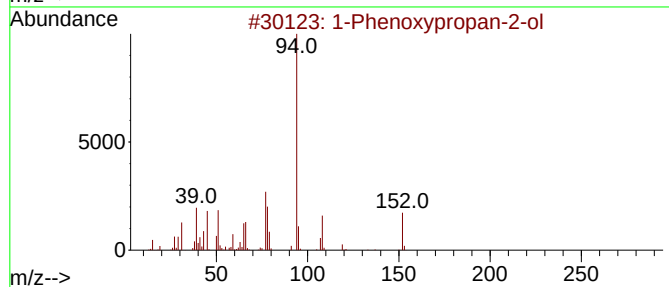
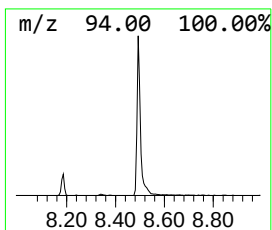
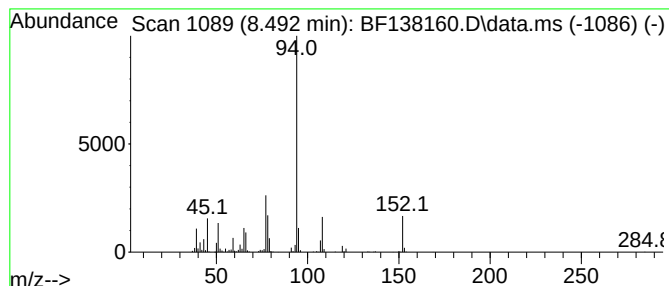
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Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	2.28 ng	305745	Naphthalene-d8	8.186

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53



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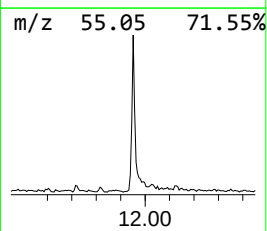
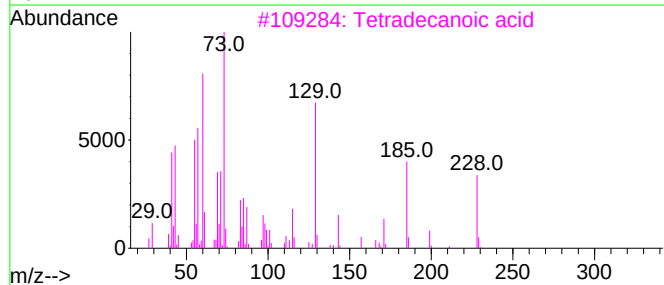
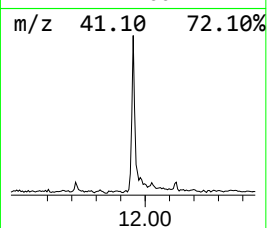
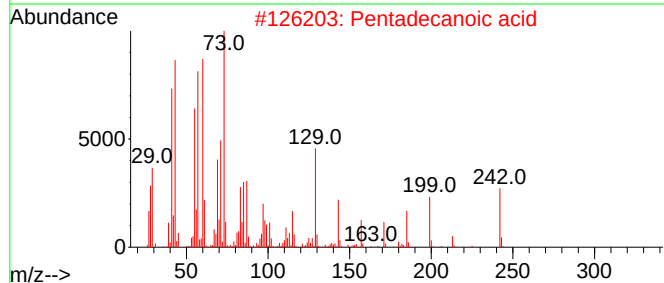
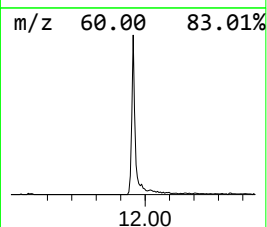
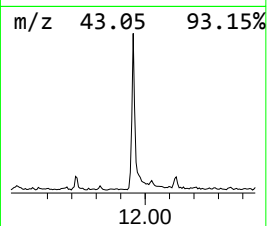
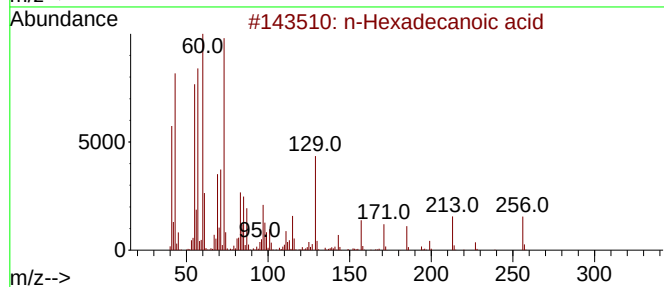
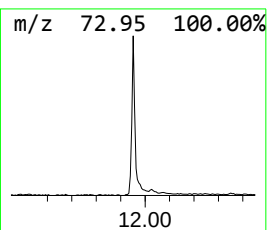
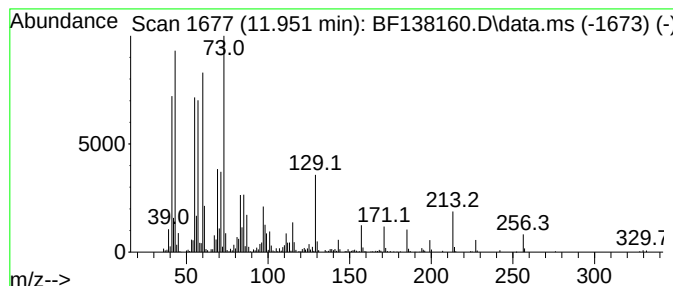
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.56 ng	523811	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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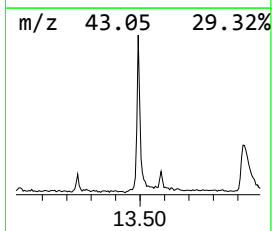
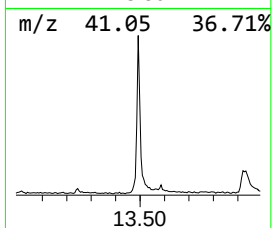
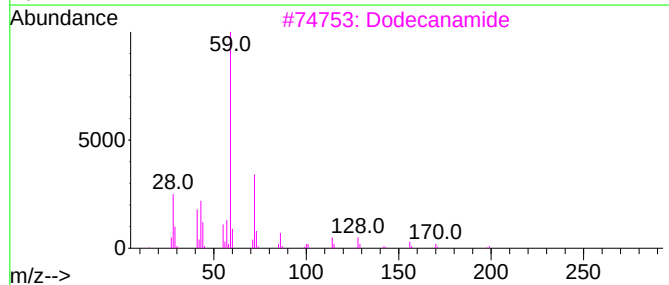
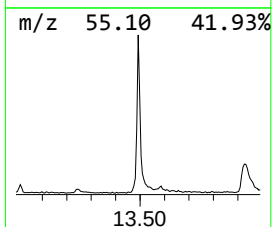
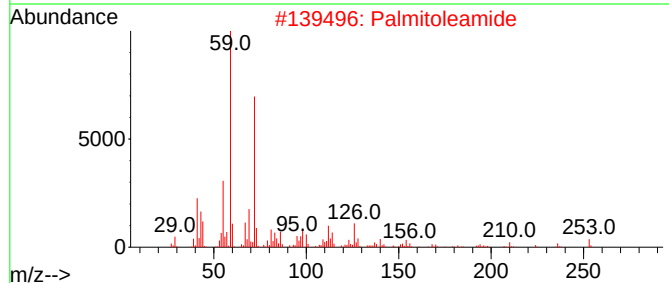
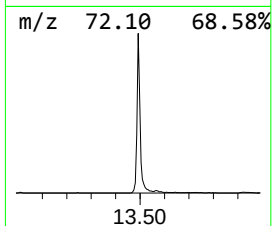
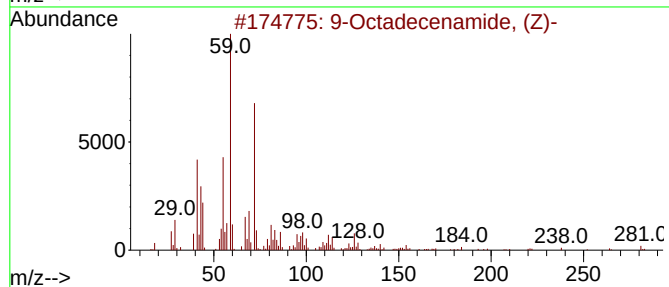
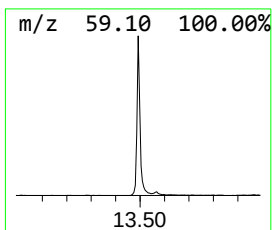
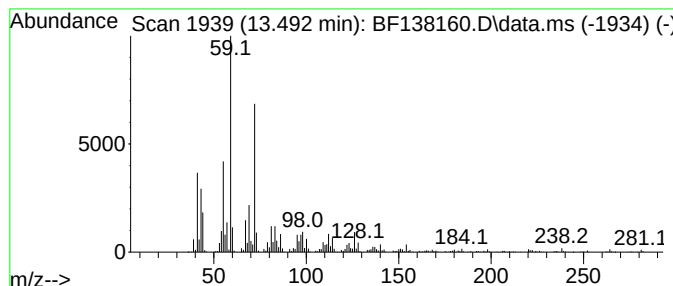
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.492	14.05 ng	1056890	Chrysene-d12		14.063	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	98
2	Palmitoleamide		253	C16H31NO	106010-22-4	78
3	Dodecanamide		199	C12H25NO	001120-16-7	53
4	Octanamide		143	C8H17NO	000629-01-6	53
5	Nonanamide		157	C9H19NO	001120-07-6	50



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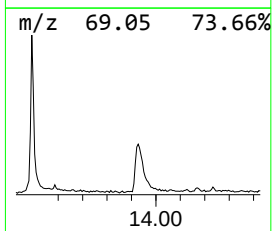
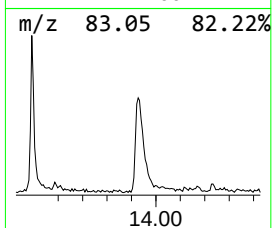
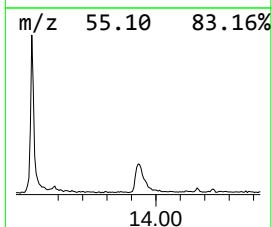
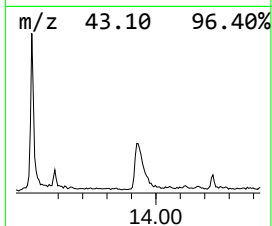
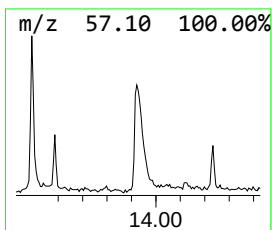
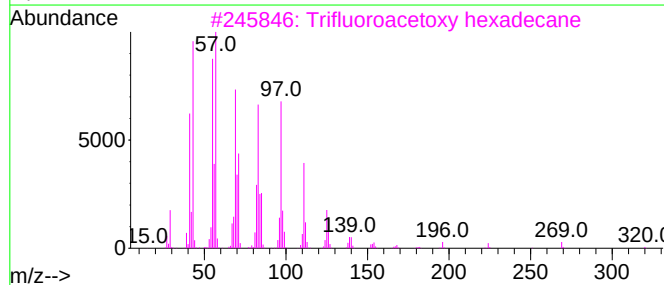
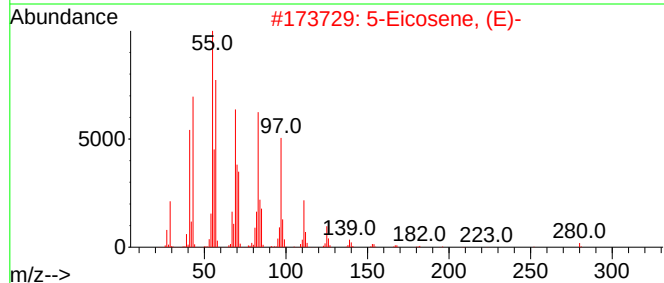
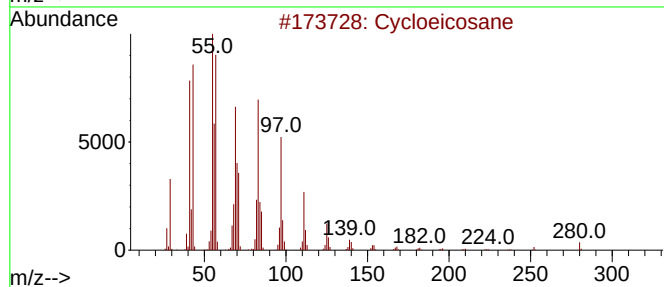
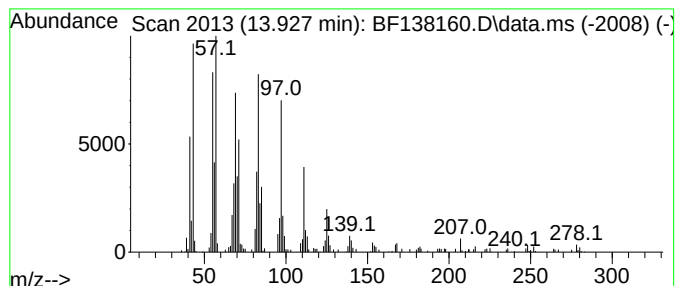
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	5.32 ng	400168	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	97
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4			1-Hexacosene	364	C26H52	018835-33-1	95
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
Data File : BF138160.D
Acq On : 07 Jun 2024 15:05
Operator : CG\JU
Sample : P2704-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPO

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.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...	2.228	60.5	ng	6068600	1	6.904	2007510	20.0
Propylene Glycol	3.434	2.9	ng	288451	1	6.904	2007510	20.0
1-Phenoxypropan...	8.492	2.3	ng	305745	2	8.186	2686800	20.0
n-Hexadecanoic ...	11.951	3.6	ng	523811	4	11.427	2939780	20.0
9-Octadecenamid...	13.492	14.1	ng	1056890	5	14.063	1504710	20.0
Cycloeicosane	13.927	5.3	ng	400168	5	14.063	1504710	20.0