

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
 Data File : BM047367.D
 Acq On : 27 Aug 2024 17:18
 Operator : RC/JU
 Sample : P3737-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-1

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_M\Methods\8270-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047367.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.257	60	63	79	rVB	192780	321669	4.01%	0.490%
2	4.563	278	285	294	rVB	147176	221999	2.77%	0.338%
3	5.010	355	361	377	rBV	2517330	3851902	47.99%	5.870%
4	6.575	620	627	639	rBV	2510153	4142697	51.61%	6.313%
5	6.981	692	696	706	rBV	94669	182528	2.27%	0.278%
6	7.351	751	759	770	rBV	854216	1324362	16.50%	2.018%
7	8.498	946	954	972	rBV	1685603	2819043	35.12%	4.296%
8	10.104	1218	1227	1234	rBV	1126605	1842847	22.96%	2.808%
9	10.869	1350	1357	1369	rBV	200502	402411	5.01%	0.613%
10	12.616	1647	1654	1670	rBV	4451466	6690743	83.35%	10.196%
11	13.727	1840	1843	1850	rVB	72643	120701	1.50%	0.184%
12	14.010	1885	1891	1898	rBV	1740619	2625891	32.71%	4.001%
13	14.074	1898	1902	1912	rVB	102390	176964	2.20%	0.270%
14	14.245	1925	1931	1933	rBV	786369	1152655	14.36%	1.756%
15	14.263	1933	1934	1941	rVB	837913	901173	11.23%	1.373%
16	15.074	2066	2072	2078	rBV2	89031	151238	1.88%	0.230%
17	15.374	2119	2123	2133	rVB	50253	92298	1.15%	0.141%
18	15.527	2142	2149	2157	rBV	3754913	5473232	68.19%	8.340%
19	15.609	2159	2163	2170	rVB3	59371	107353	1.34%	0.164%
20	15.768	2185	2190	2199	rBV5	55457	113358	1.41%	0.173%
21	16.439	2300	2304	2313	rVB	82562	141937	1.77%	0.216%
22	16.521	2313	2318	2323	rBV4	58344	121343	1.51%	0.185%
23	16.598	2328	2331	2340	rVB	70805	143210	1.78%	0.218%
24	16.780	2356	2362	2366	rBV	2180939	3078070	38.35%	4.690%
25	16.821	2366	2369	2375	rVB	1241777	1552519	19.34%	2.366%
26	16.909	2380	2384	2391	rVV	335088	489866	6.10%	0.746%
27	16.986	2392	2397	2402	rVB3	47872	90773	1.13%	0.138%
28	17.198	2430	2433	2436	rBV	80574	95135	1.19%	0.145%
29	17.309	2448	2452	2457	rBV3	63597	90473	1.13%	0.138%
30	17.486	2478	2482	2489	rVB2	100177	145745	1.82%	0.222%
31	17.656	2507	2511	2515	rBV	212136	317070	3.95%	0.483%
32	17.709	2516	2520	2529	rVV2	805005	1339006	16.68%	2.040%
33	17.786	2530	2533	2539	rVV	145610	256383	3.19%	0.391%
34	17.851	2539	2544	2548	rVV3	302690	553957	6.90%	0.844%
35	17.886	2548	2550	2559	rVB	150189	228276	2.84%	0.348%
36	18.168	2595	2598	2602	rVB	127816	154438	1.92%	0.235%

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37	18.215	2603	2606	2611	rVB	96905	122784	1.53%	0.187%
38	18.592	2666	2670	2674	rBV	117129	182878	2.28%	0.279%
39	18.739	2691	2695	2703	rBV3	115953	197071	2.46%	0.300%
40	18.856	2710	2715	2721	rBV	2078970	2838738	35.37%	4.326%
41	19.015	2738	2742	2747	rBV2	277904	377509	4.70%	0.575%
42	19.227	2769	2778	2787	rBV2	1781440	2913156	36.29%	4.439%
43	19.450	2811	2816	2820	rVB	6550272	8026958	100.00%	12.232%
44	20.168	2934	2938	2942	rVB	869831	954418	11.89%	1.454%
45	20.492	2991	2993	2998	rVB	199225	221615	2.76%	0.338%
46	20.756	3035	3038	3042	rVB2	426631	487800	6.08%	0.743%
47	21.021	3077	3083	3087	rBV2	2009470	3664791	45.66%	5.585%
48	21.062	3087	3090	3095	rVB	801689	967741	12.06%	1.475%
49	22.880	3395	3399	3405	rBV	517897	1132861	14.11%	1.726%
50	23.721	3537	3542	3549	rVB	1000772	2022614	25.20%	3.082%

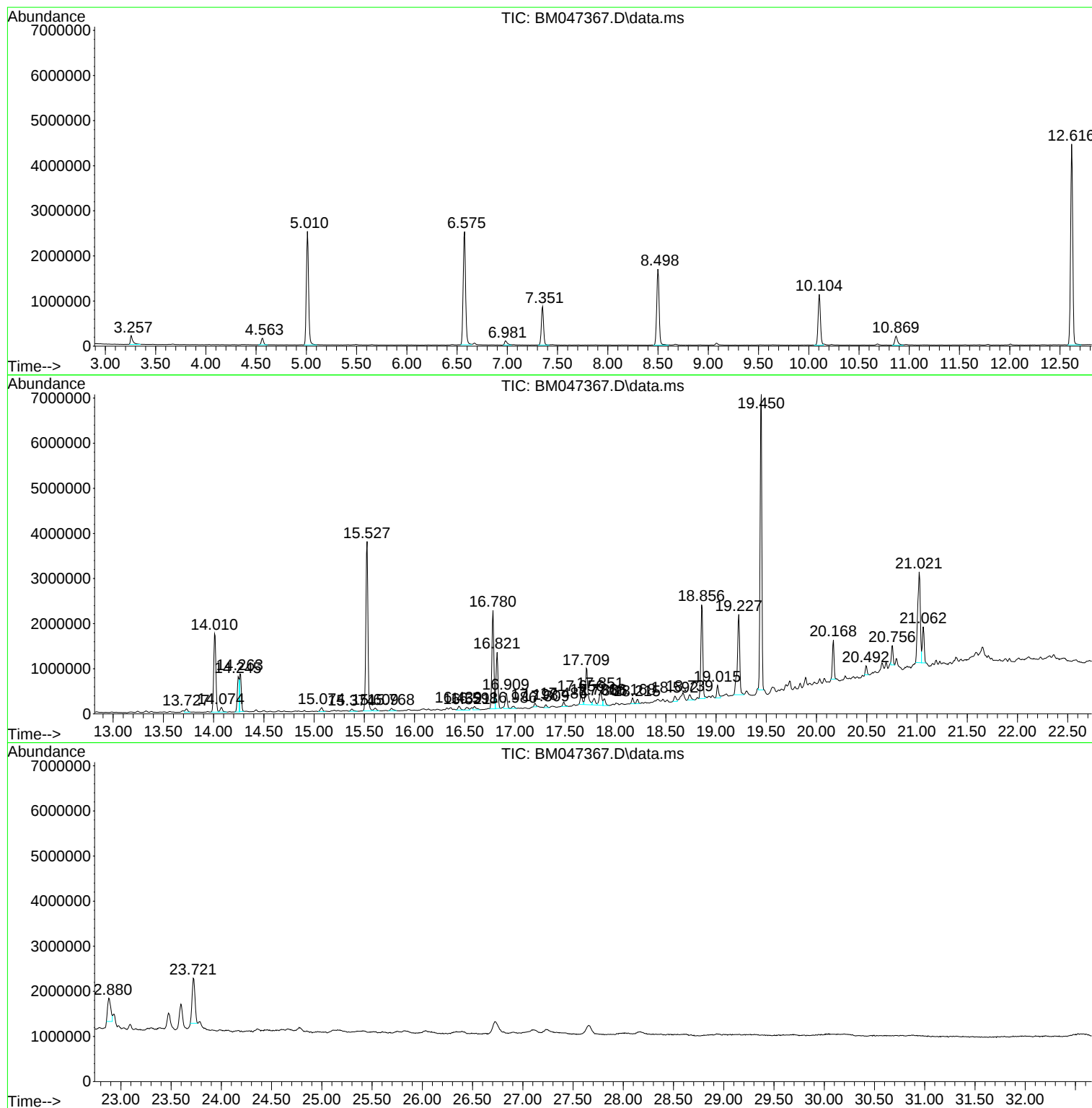
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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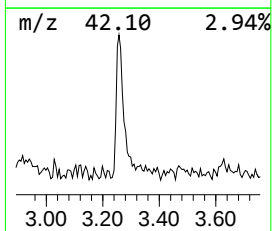
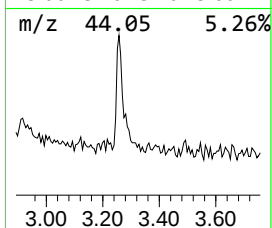
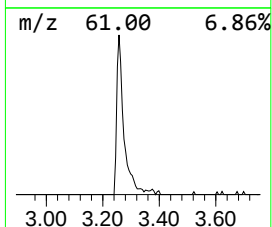
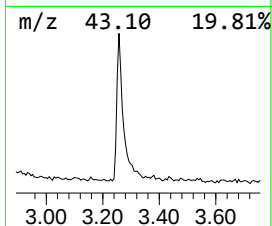
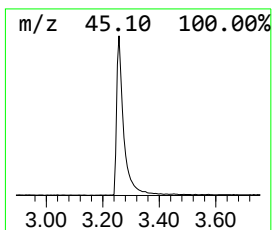
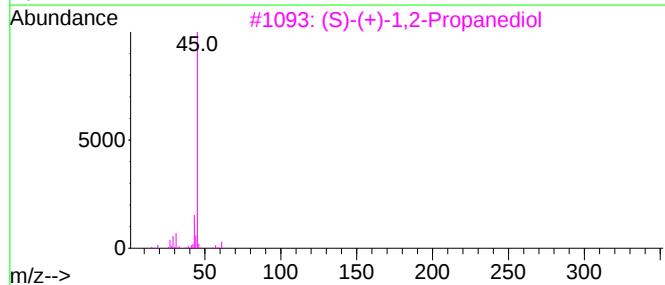
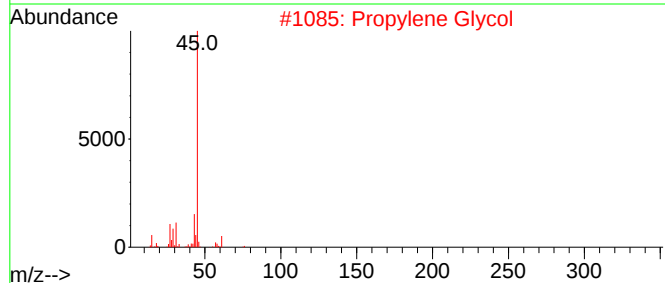
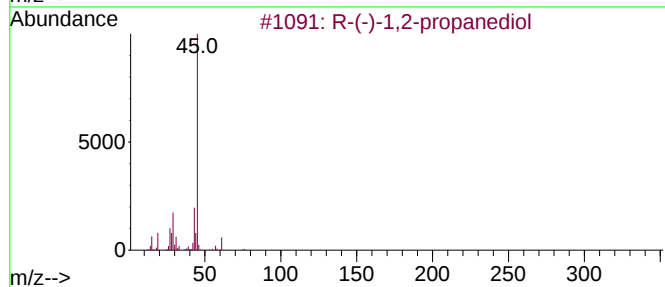
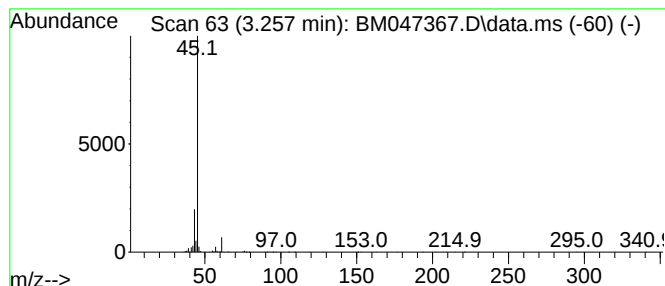
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	4.86 ng	321669	1,4-Dichlorobenzene-d4	7.351

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
2		Propylene Glycol	76	C3H8O2	000057-55-6	78
3		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5		Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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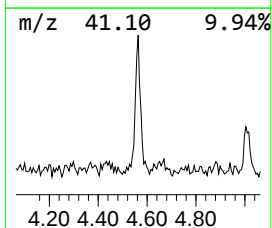
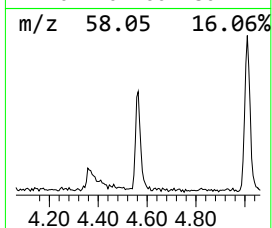
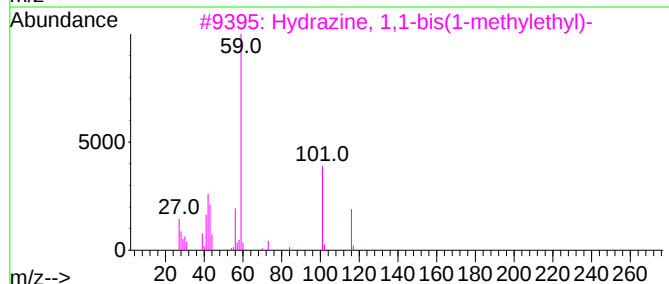
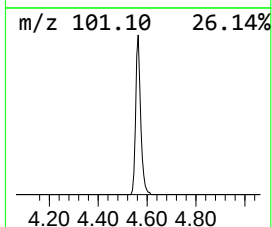
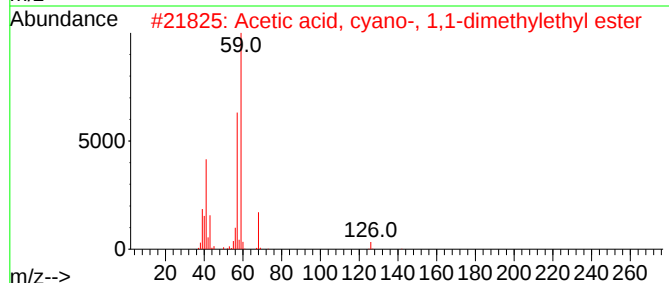
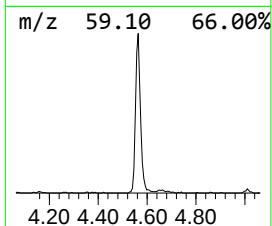
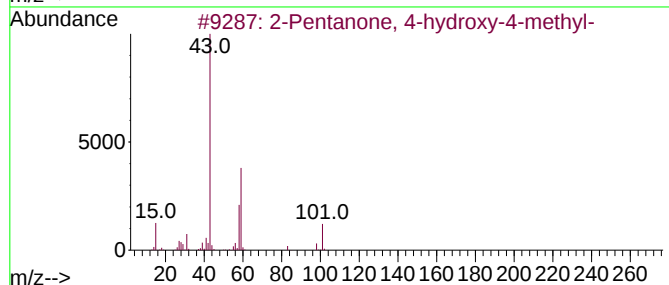
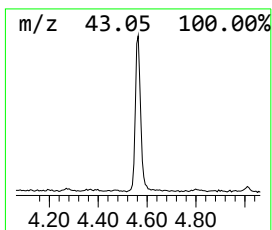
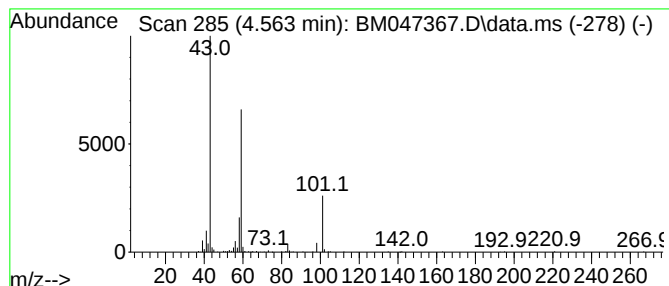
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	3.35 ng	221999	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			Tetraglyme	222	C10H22O5	000143-24-8	23



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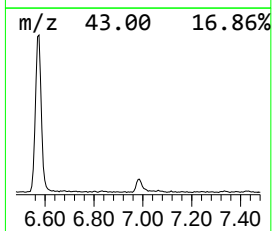
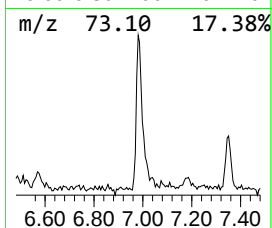
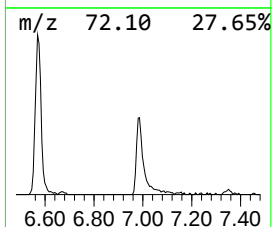
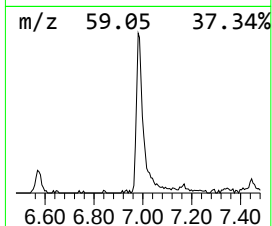
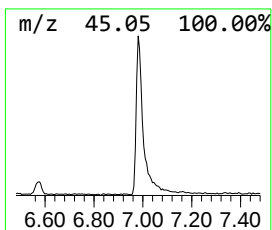
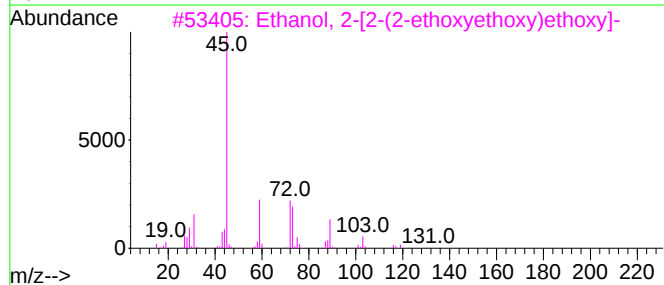
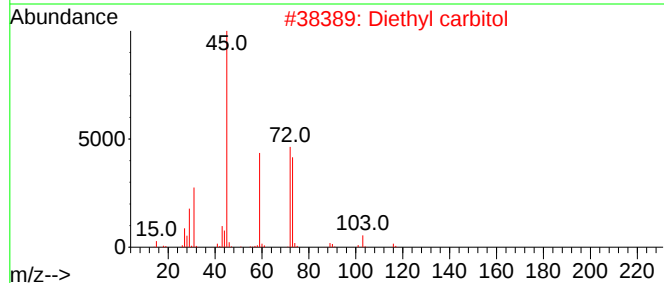
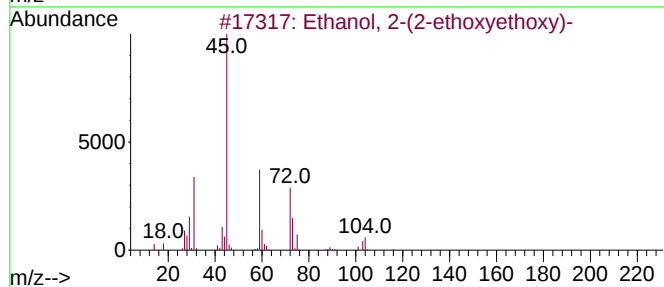
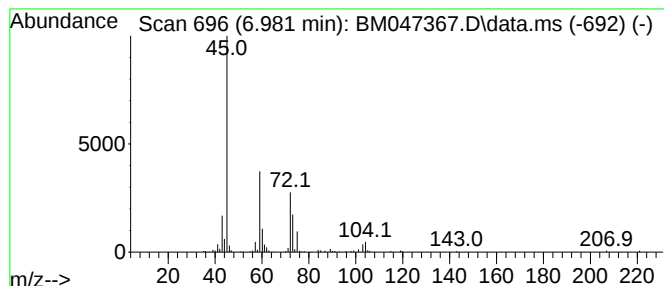
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.981	2.76 ng	182528	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	64
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	56
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42



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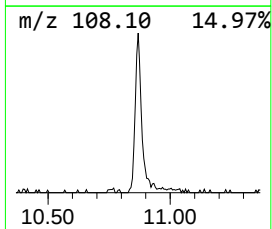
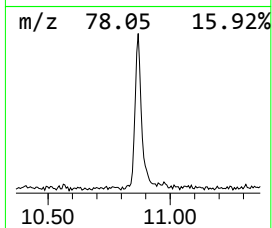
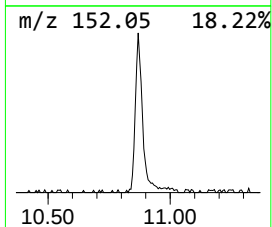
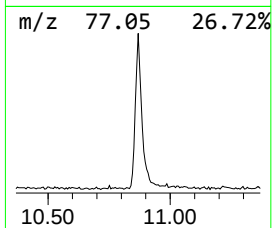
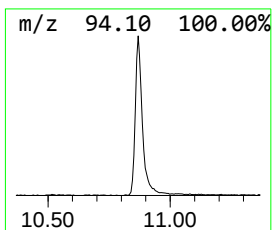
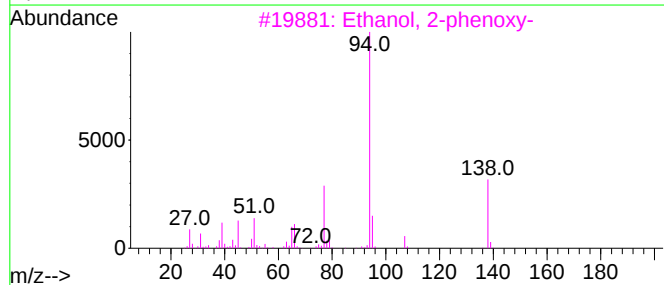
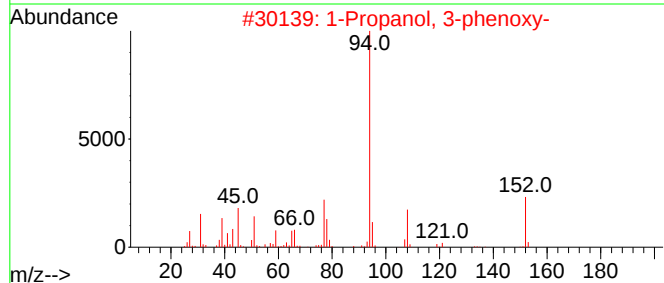
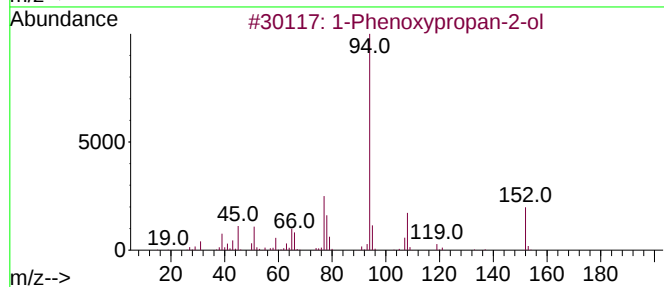
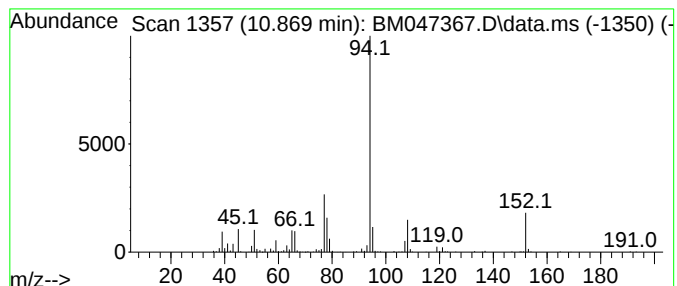
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	4.37 ng	402411	Naphthalene-d8	10.104

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	83
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



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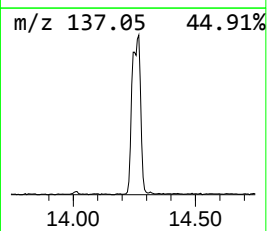
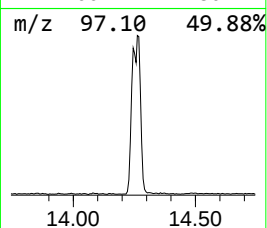
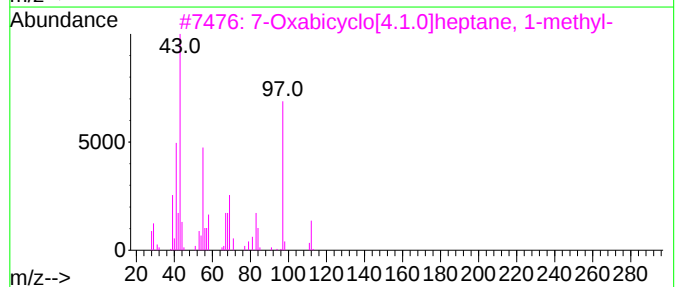
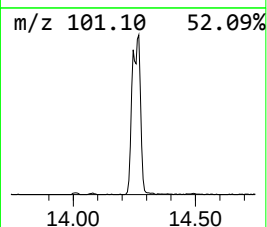
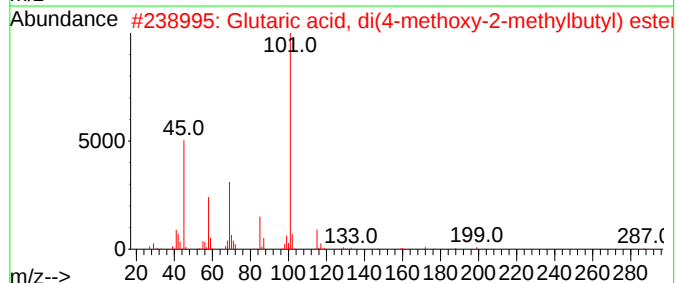
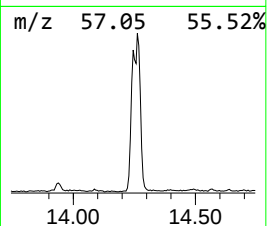
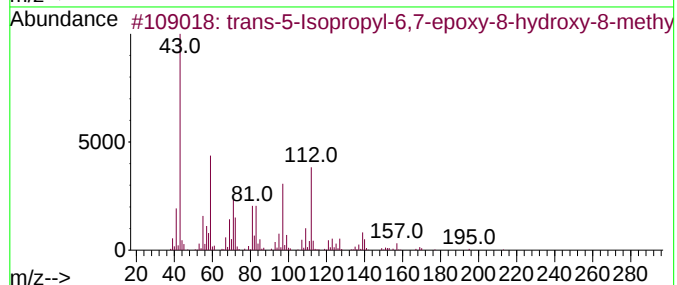
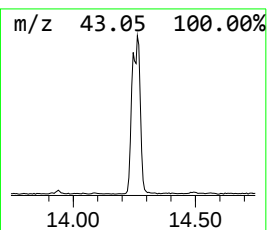
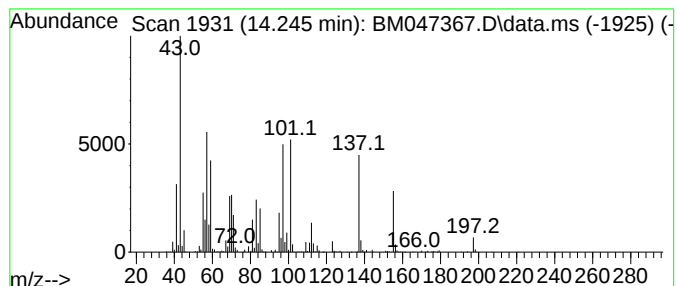
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.245 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	8.78 ng	1152660	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
2			Glutaric acid, di(4-methoxy-2-me...	332	C17H32O6	1010359-42-1	10
3			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5			Acetic acid, cyano(hydroxyimino)...	170	C7H10N2O3	076101-98-9	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047367.D
Acq On : 27 Aug 2024 17:18
Operator : RC/JU
Sample : P3737-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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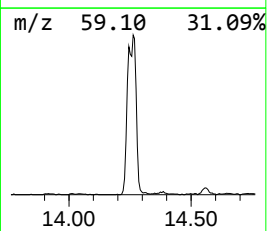
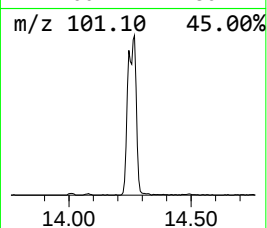
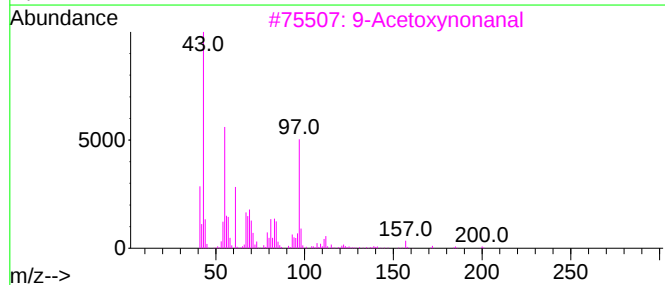
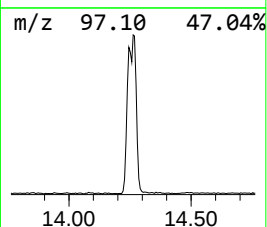
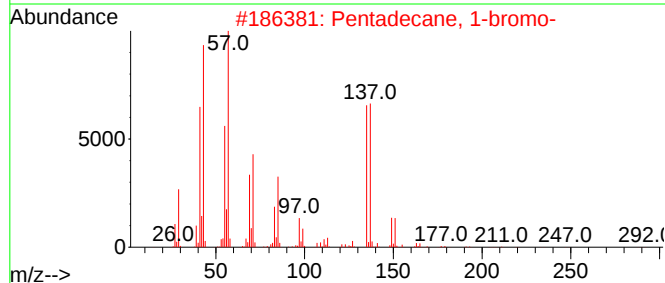
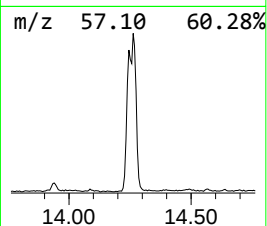
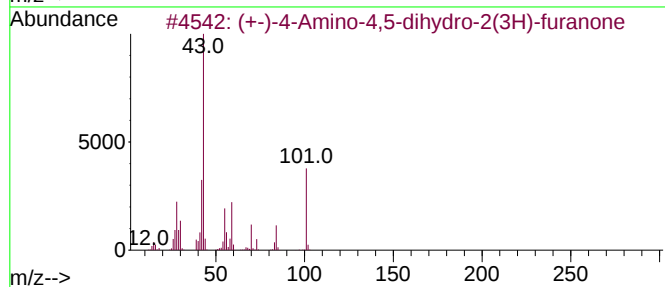
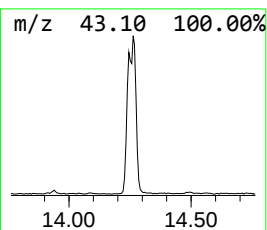
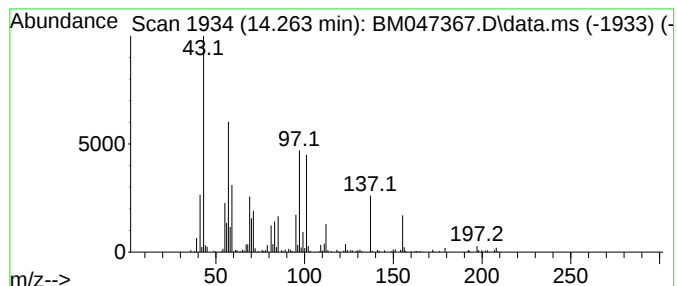
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.262 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.262	6.86 ng	901173	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	14		
2	Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	14		
3	9-Acetoxynonanal	200	C11H20O3	029541-97-7	11		
4	Nonane, 2-bromo-5-ethyl-	234	C11H23Br	055162-38-4	10		
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047367.D
Acq On : 27 Aug 2024 17:18
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Sample : P3737-01
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ClientSampleId :
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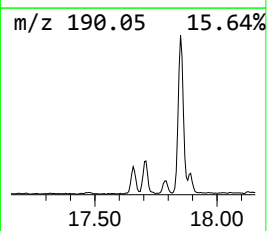
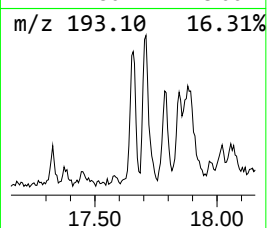
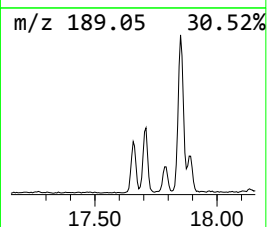
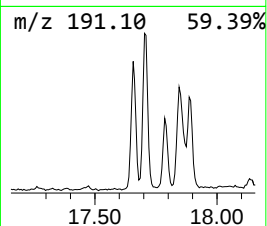
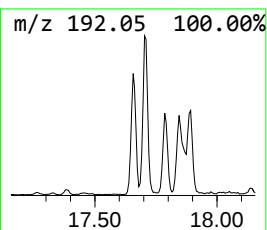
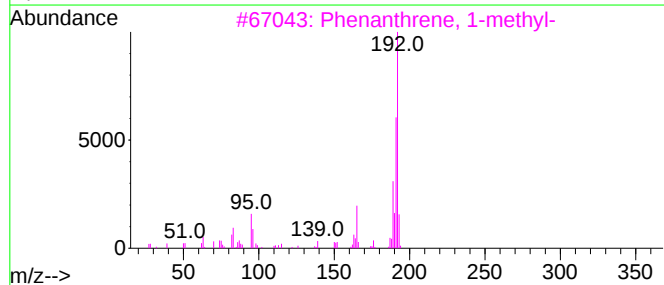
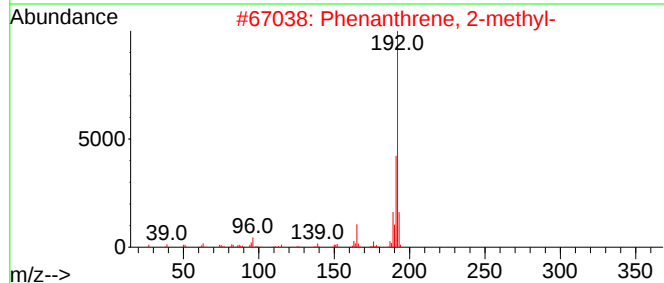
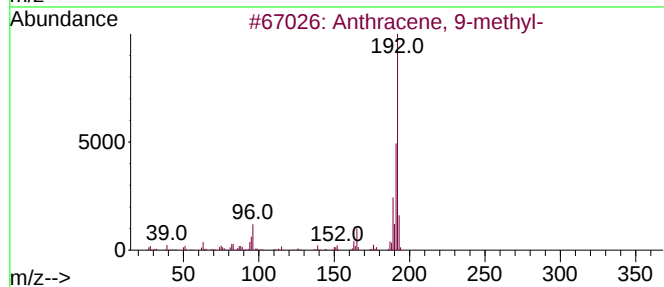
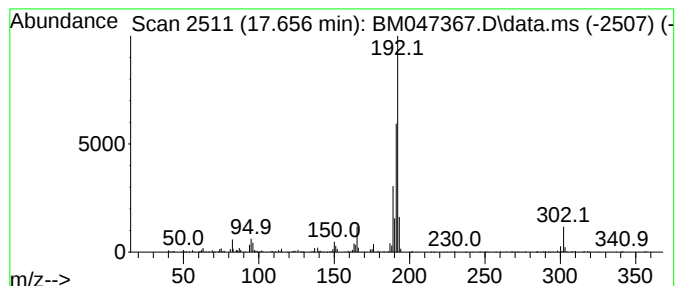
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Anthracene, 9-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.656	2.06 ng	317070	Phenanthrene-d10	16.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-methyl-	192	C15H12	000779-02-2	96
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
4			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	93
5			Anthracene, 2-methyl-	192	C15H12	000613-12-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047367.D
Acq On : 27 Aug 2024 17:18
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Sample : P3737-01
Misc :
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Instrument :
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ClientSampleId :
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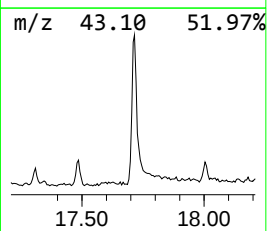
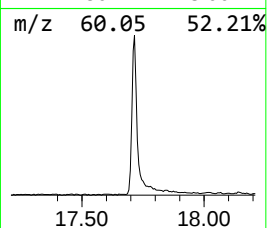
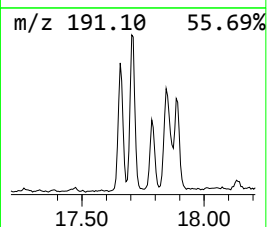
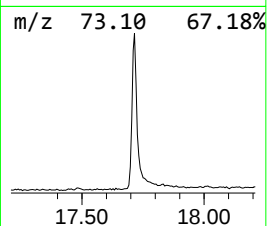
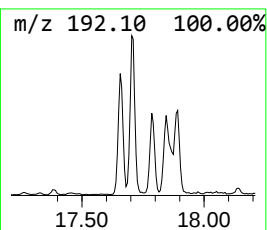
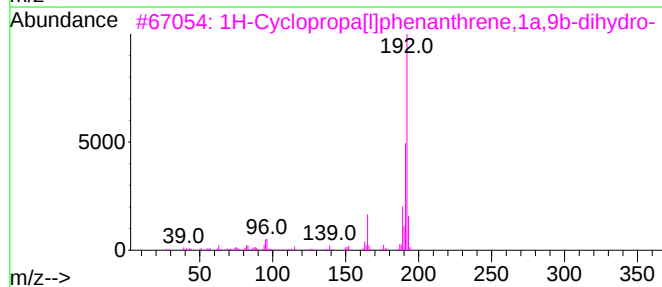
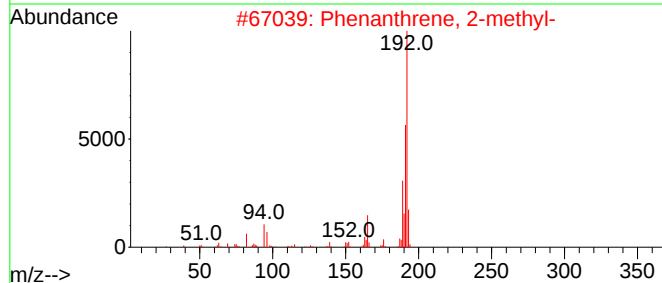
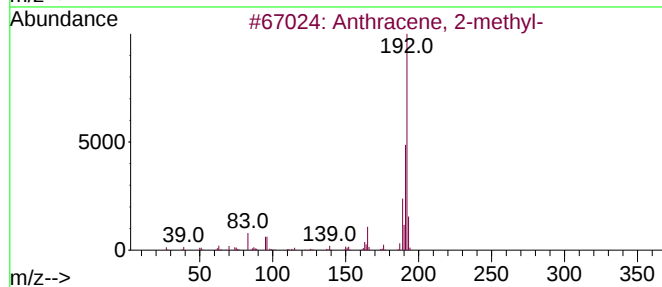
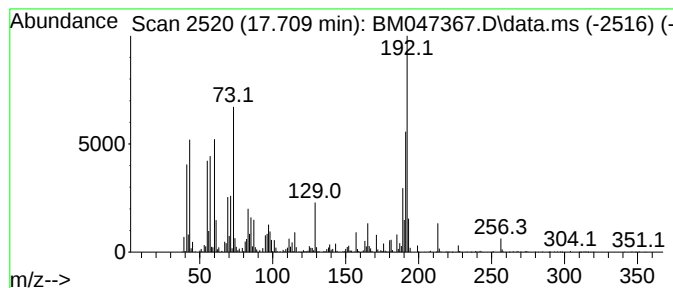
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Anthracene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.709	8.70 ng	1339010	Phenanthrene-d10	16.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3			1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
4			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047367.D
Acq On : 27 Aug 2024 17:18
Operator : RC/JU
Sample : P3737-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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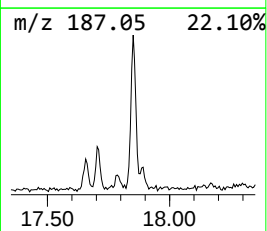
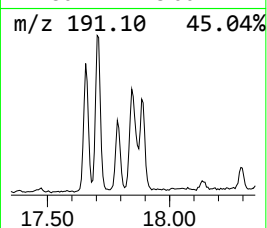
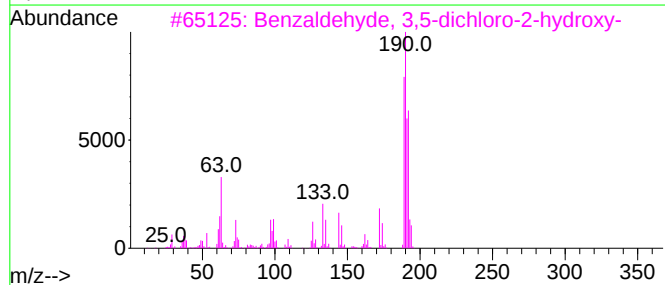
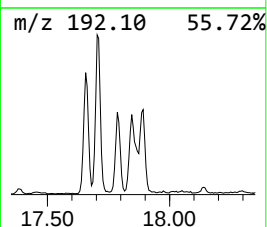
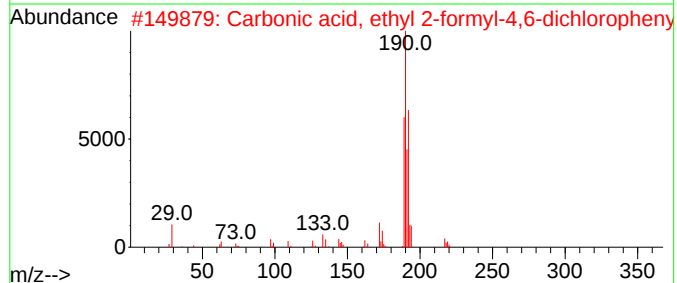
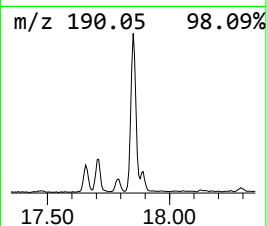
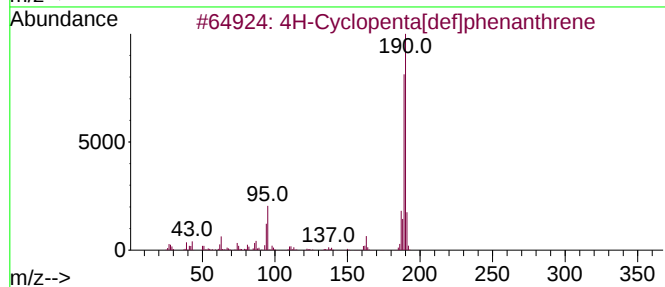
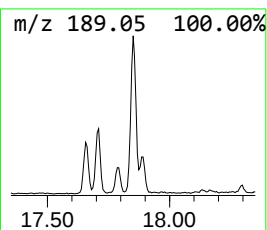
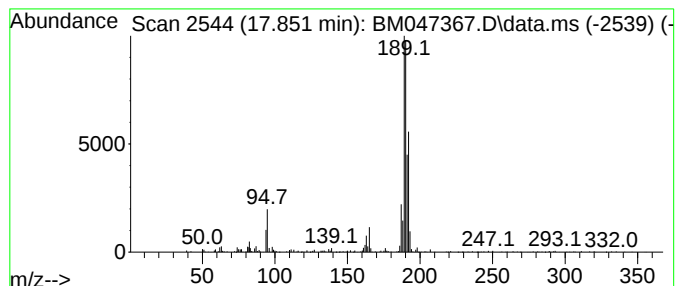
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.851	3.60 ng	553957	Phenanthrene-d10	16.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	83
2			Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
4			Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	43
5			2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
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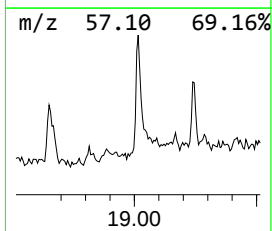
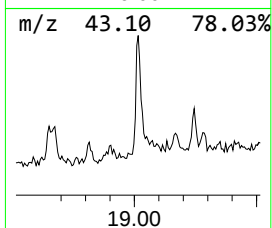
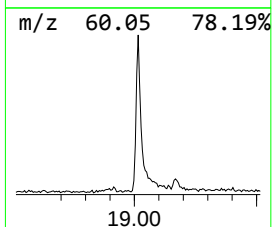
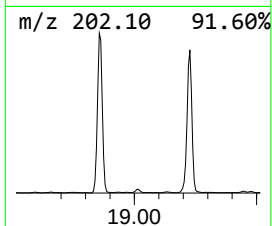
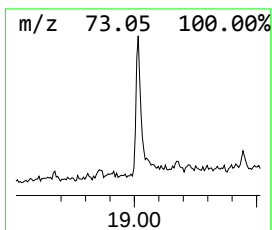
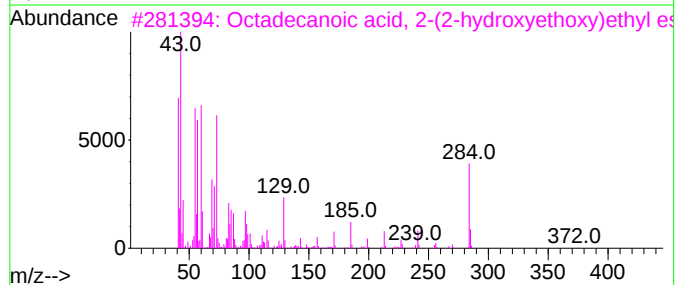
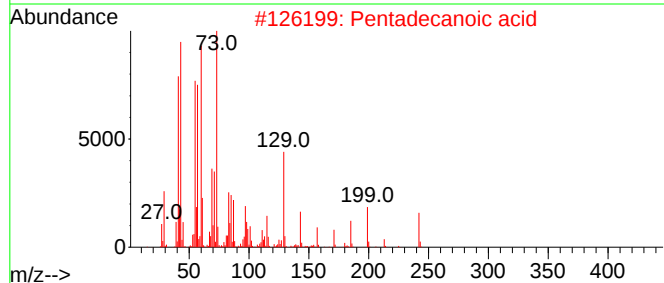
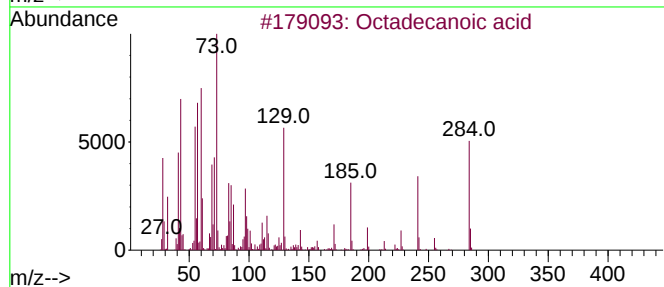
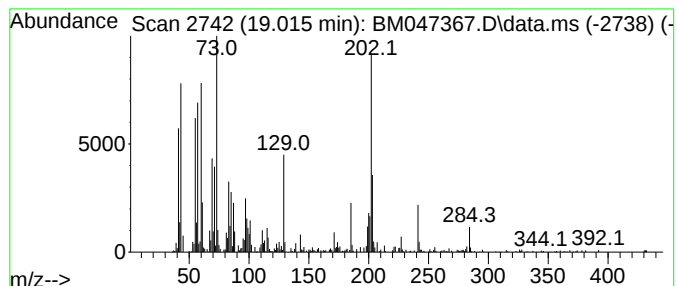
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.015	2.06 ng	377509	Chrysene-d12	21.021	
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	89
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	52
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047367.D
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Instrument :
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ClientSampleId :
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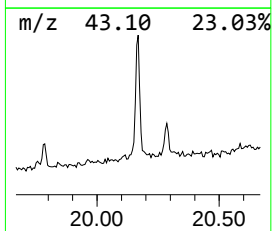
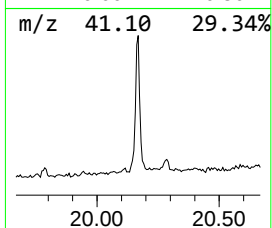
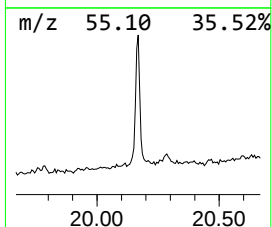
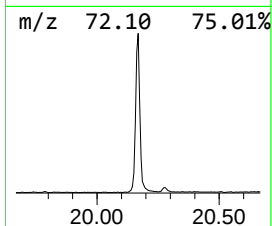
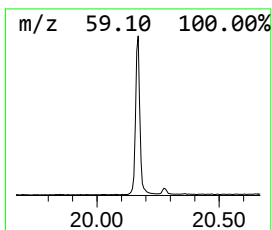
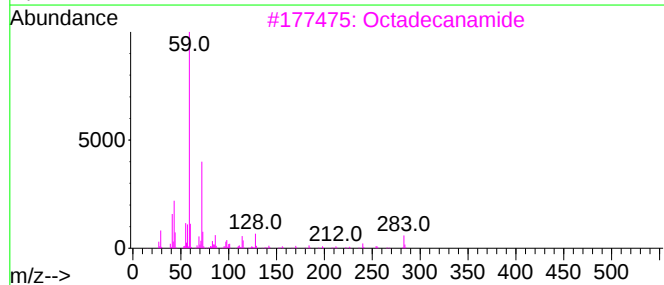
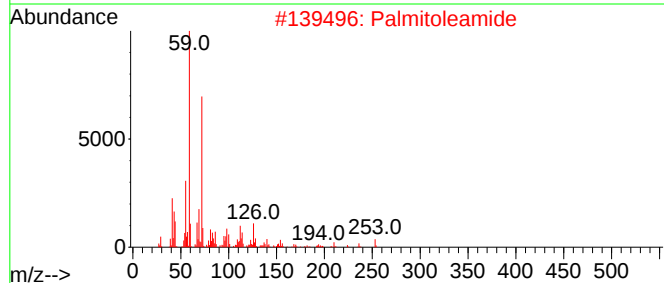
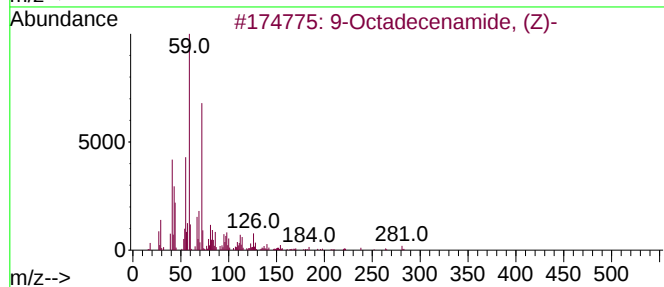
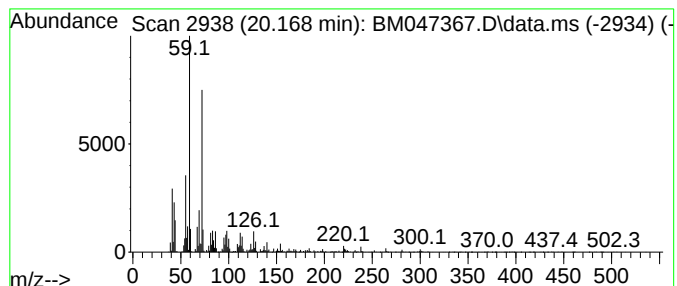
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.168	5.21 ng	954418	Chrysene-d12	21.021

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Palmitoleamide	253	C16H31NO	106010-22-4	80
3		Octadecanamide	283	C18H37NO	000124-26-5	53
4		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47
5		2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047367.D
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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-1

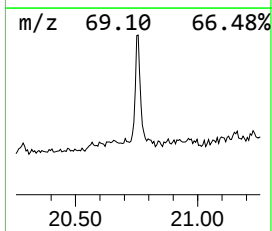
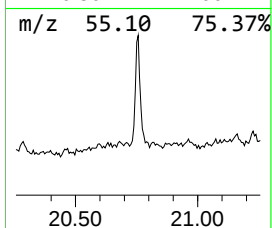
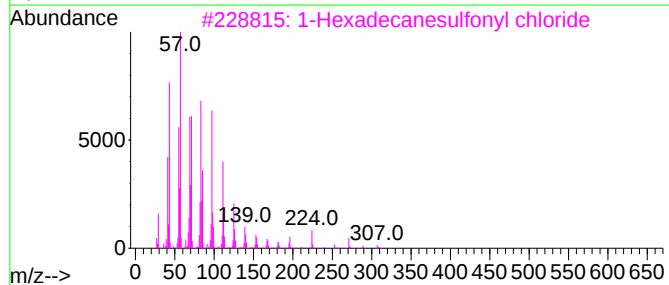
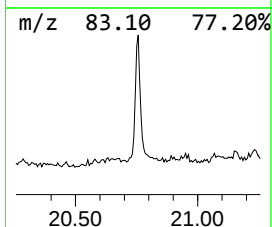
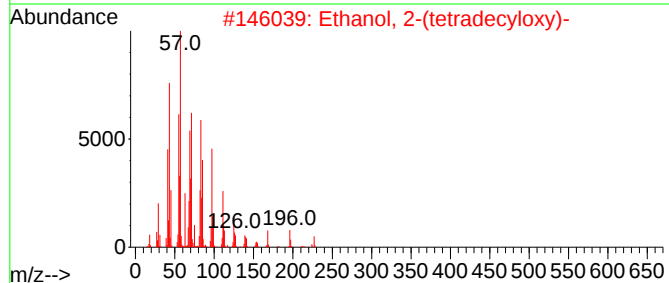
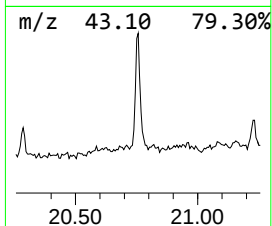
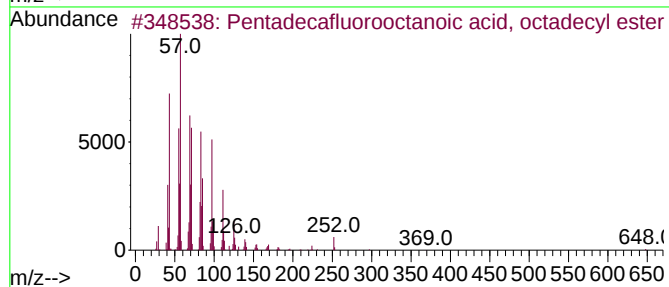
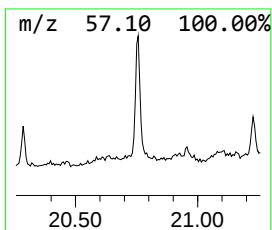
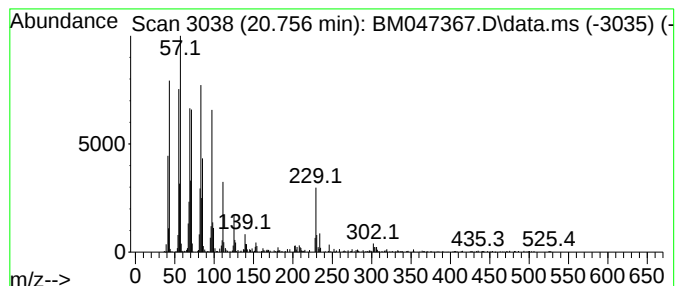
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentadecafluorooctanoic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	2.66 ng	487800	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3			1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
5			2-Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082724\
Data File : BM047367.D
Acq On : 27 Aug 2024 17:18
Operator : RC/JU
Sample : P3737-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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
R-(-)-1,2-propa...	3.257	4.9	ng	321669	1	7.351	1324360	20.0
2-Pentanone, 4-...	4.563	3.4	ng	221999	1	7.351	1324360	20.0
Ethanol, 2-(2-e...	6.981	2.8	ng	182528	1	7.351	1324360	20.0
1-Phenoxypropan...	10.869	4.4	ng	402411	2	10.104	1842850	20.0
unknown14.245	14.245	8.8	ng	1152660	3	14.010	2625890	20.0
unknown14.262	14.262	6.9	ng	901173	3	14.010	2625890	20.0
Anthracene, 9-m...	17.656	2.1	ng	317070	4	16.780	3078070	20.0
Anthracene, 2-m...	17.709	8.7	ng	1339010	4	16.780	3078070	20.0
4H-Cyclopenta[d...	17.851	3.6	ng	553957	4	16.780	3078070	20.0
Octadecanoic acid	19.015	2.1	ng	377509	5	21.021	3664790	20.0
9-Octadecenamid...	20.168	5.2	ng	954418	5	21.021	3664790	20.0
Pentadecafluoro...	20.756	2.7	ng	487800	5	21.021	3664790	20.0