

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
 Data File : BM047301.D
 Acq On : 21 Aug 2024 17:06
 Operator : RC/JU
 Sample : P3617-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 VCPS-B5-081424-10-14

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047301.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	75	rBV	151628	229818	2.86%	0.422%
2	4.563	279	285	294	rVB	174593	251553	3.13%	0.462%
3	5.010	355	361	372	rBV	2600975	3797233	47.18%	6.967%
4	6.569	615	626	641	rBV	2549527	4074927	50.63%	7.477%
5	7.351	750	759	769	rBV	753582	1177690	14.63%	2.161%
6	8.498	947	954	964	rBV	1635655	2743783	34.09%	5.034%
7	9.087	1049	1054	1062	rBV	58185	98571	1.22%	0.181%
8	10.110	1220	1228	1235	rBV	953274	1577864	19.61%	2.895%
9	10.875	1352	1358	1371	rBV	124112	274938	3.42%	0.504%
10	11.086	1386	1394	1403	rBV3	33521	92698	1.15%	0.170%
11	12.622	1647	1655	1672	rBV	3775539	5724505	71.13%	10.503%
12	14.016	1885	1892	1899	rBV	1435624	2171437	26.98%	3.984%
13	14.269	1926	1935	1942	rBV2	73173	169219	2.10%	0.310%
14	14.569	1979	1986	1996	rBV2	56667	192023	2.39%	0.352%
15	15.521	2142	2148	2169	rBV	3548556	5254570	65.29%	9.641%
16	16.780	2356	2362	2366	rBV	1914333	2704021	33.60%	4.961%
17	16.821	2366	2369	2376	rVV	361225	491424	6.11%	0.902%
18	16.910	2380	2384	2392	rVB	109271	159170	1.98%	0.292%
19	17.715	2515	2521	2530	rBV2	767773	1153717	14.34%	2.117%
20	17.845	2540	2543	2548	rBV2	71807	105978	1.32%	0.194%
21	18.856	2710	2715	2720	rBV	805796	1118597	13.90%	2.052%
22	19.015	2738	2742	2752	rBV2	327143	506430	6.29%	0.929%
23	19.156	2761	2766	2770	rBV	813706	936877	11.64%	1.719%
24	19.221	2770	2777	2786	rVB	651161	1089275	13.53%	1.999%
25	19.445	2810	2815	2819	rBV	6640344	8047913	100.00%	14.766%
26	19.480	2819	2821	2826	rVB	287994	288583	3.59%	0.529%
27	19.733	2861	2864	2868	rVB2	111432	133965	1.66%	0.246%
28	19.833	2878	2881	2885	rVB	104812	118487	1.47%	0.217%
29	20.756	3034	3038	3050	rVB3	471740	790618	9.82%	1.451%
30	21.015	3076	3082	3087	rBV2	2548902	3884206	48.26%	7.127%
31	21.056	3087	3089	3099	rVB	429825	548653	6.82%	1.007%
32	22.056	3255	3259	3264	rVB	230575	336516	4.18%	0.617%
33	22.303	3297	3301	3309	rVB3	400543	652608	8.11%	1.197%
34	22.874	3394	3398	3404	rBV	221781	445549	5.54%	0.817%
35	23.709	3533	3540	3557	rVB	1300764	3158407	39.25%	5.795%

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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-BM081024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

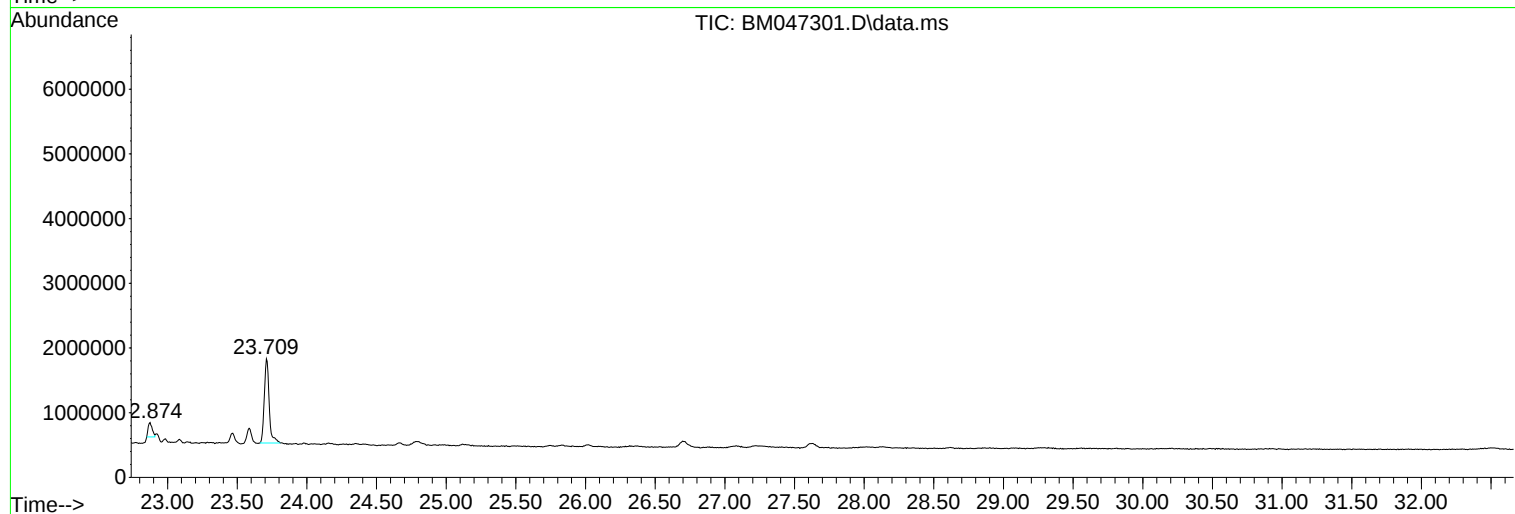
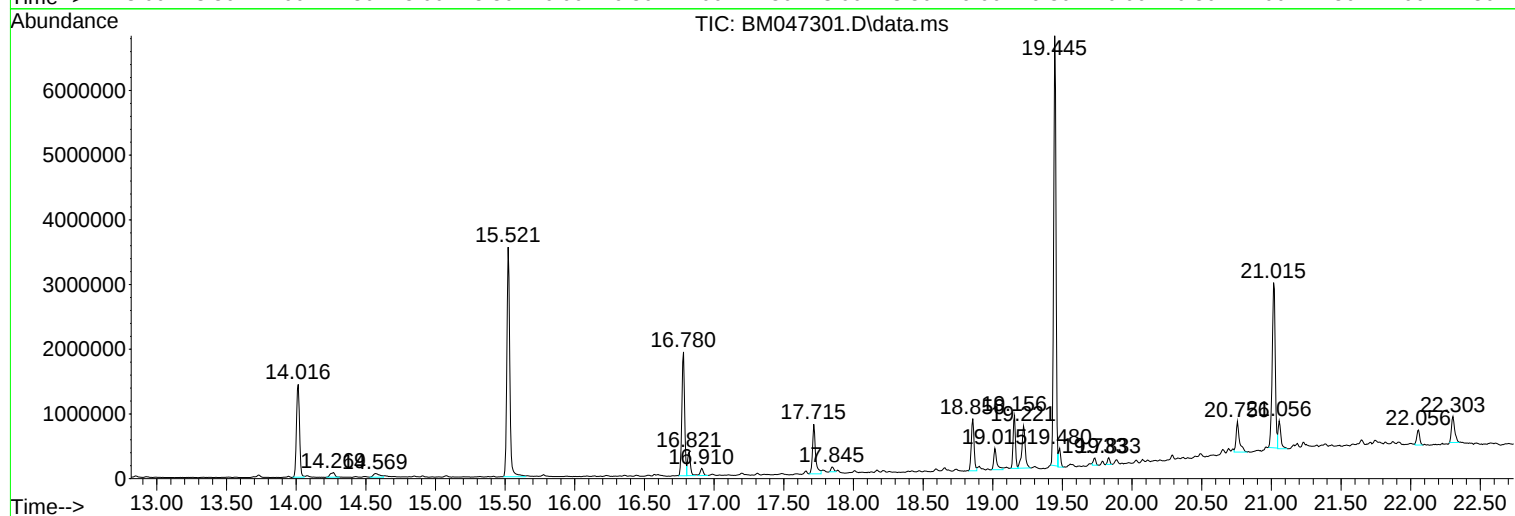
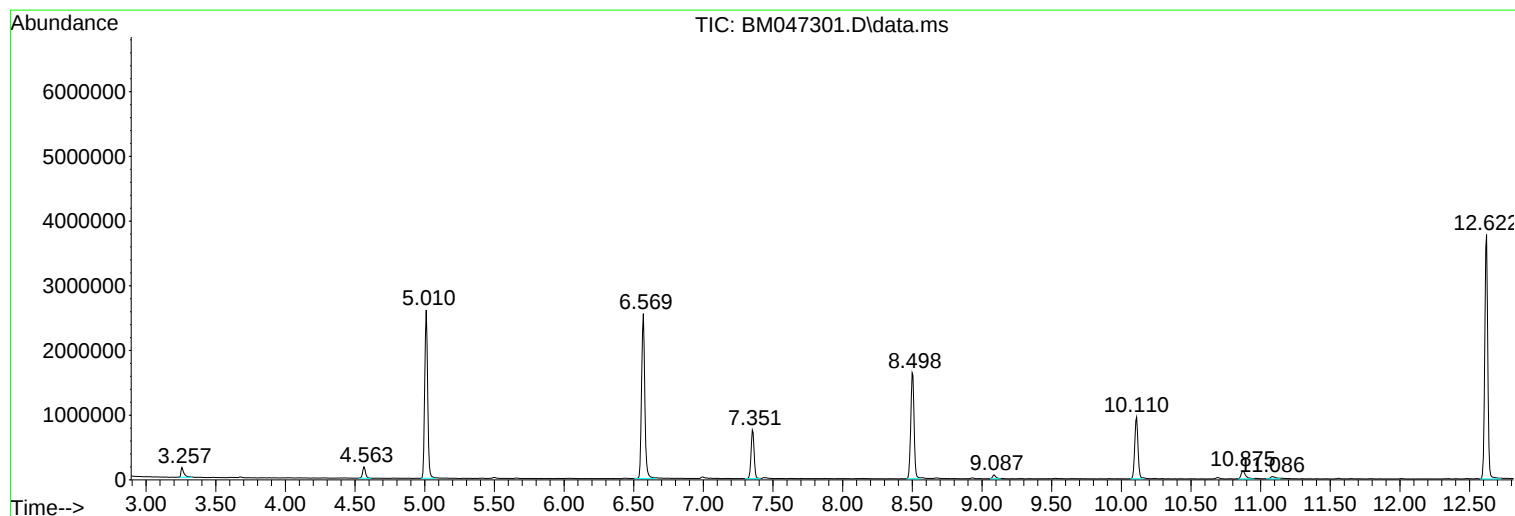
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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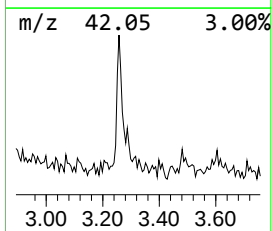
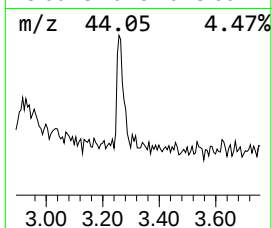
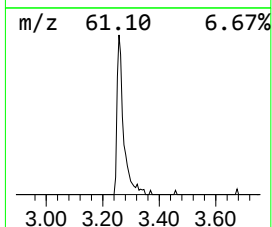
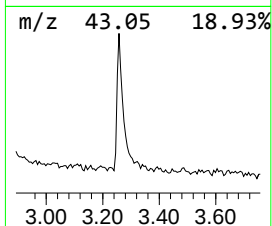
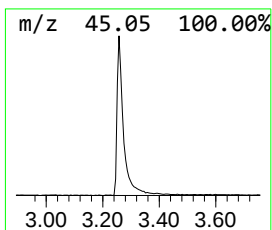
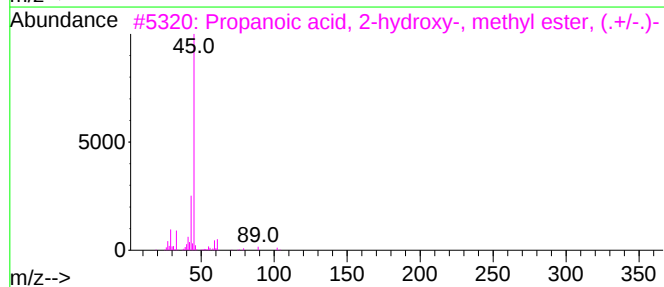
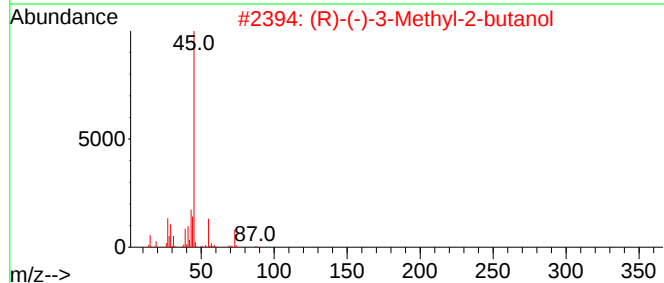
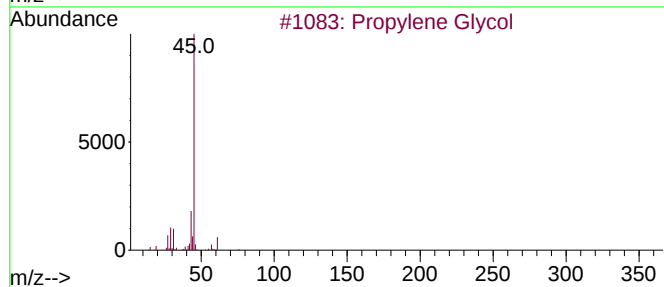
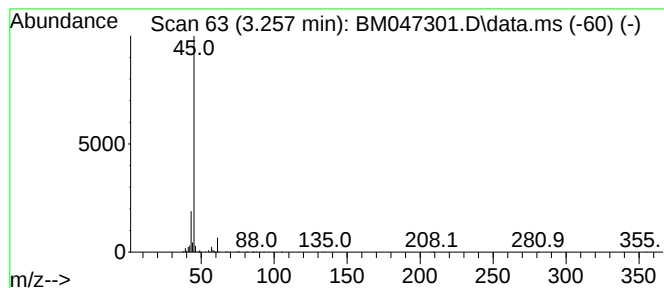
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.257	3.90 ng	229818	1,4-Dichlorobenzene-d4	7.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	50
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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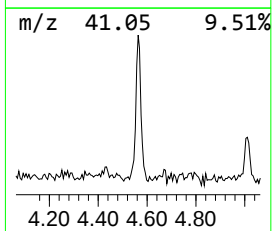
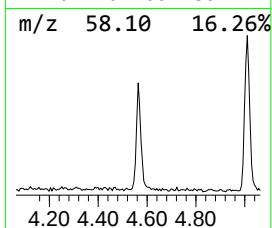
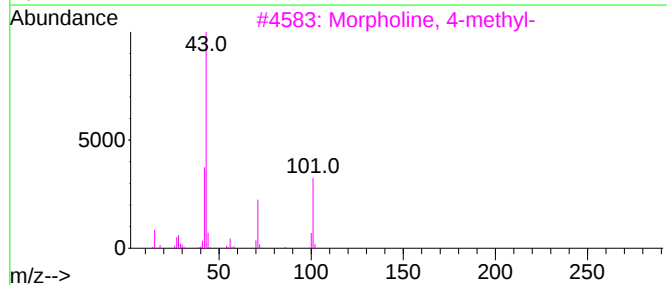
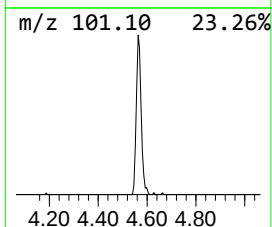
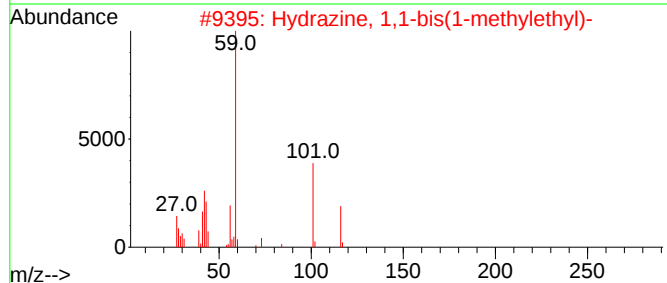
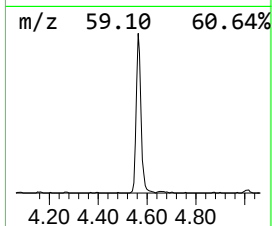
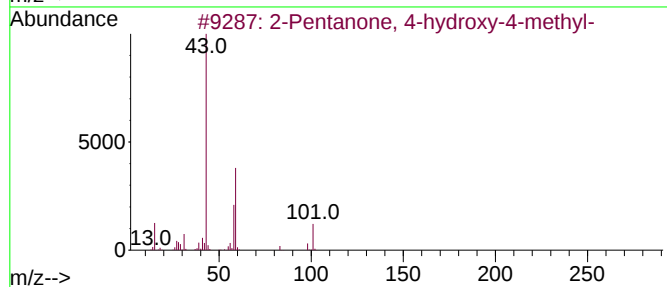
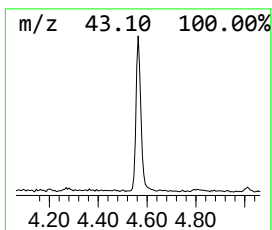
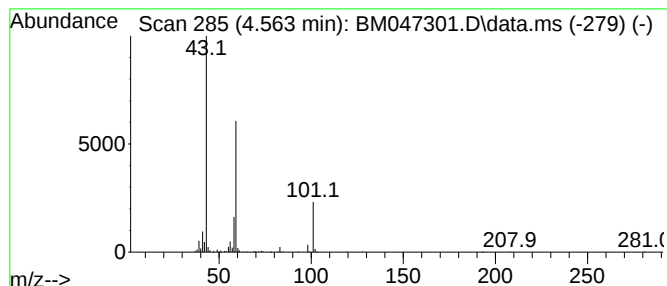
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	4.27 ng	251553	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	50
2		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Silane, dimethyl-	60	C2H8Si	001111-74-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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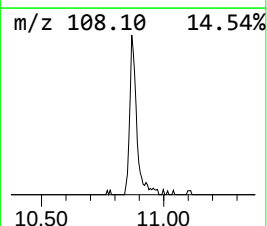
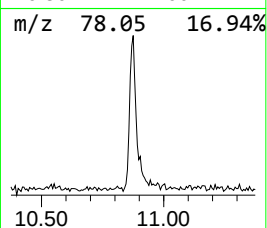
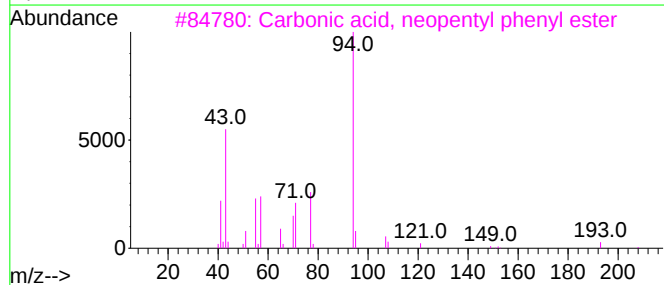
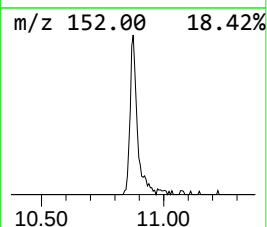
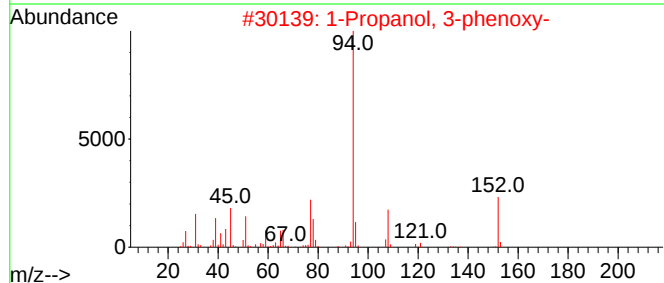
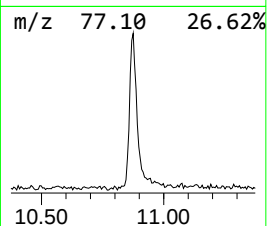
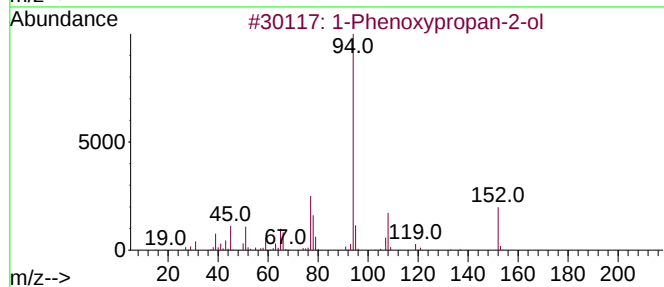
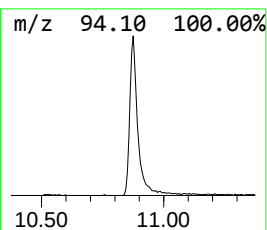
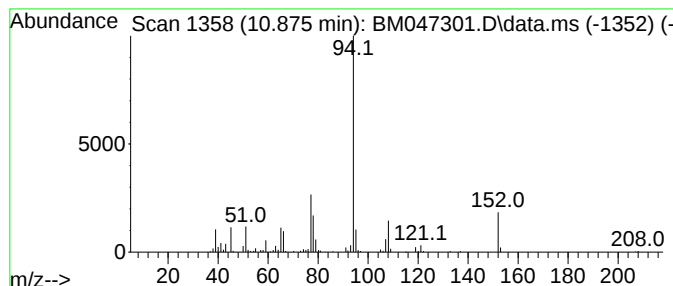
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	3.48 ng	274938	Naphthalene-d8	10.110

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			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5			1-Amino-3-phenoxypropan-2-ol	167	C9H13NO2	004287-19-8	64



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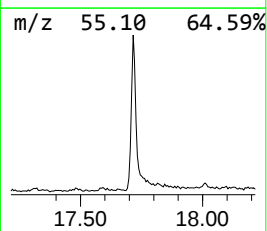
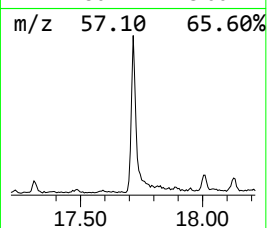
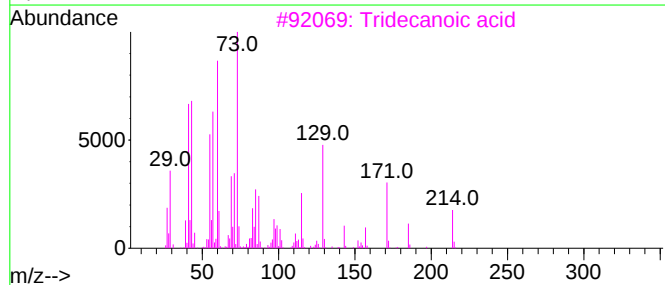
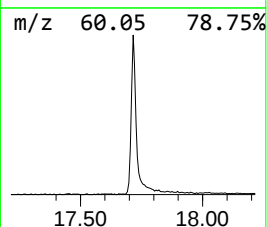
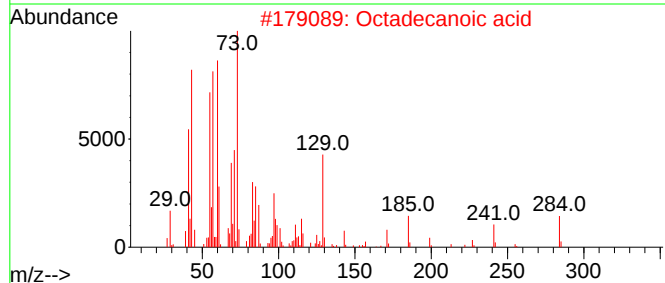
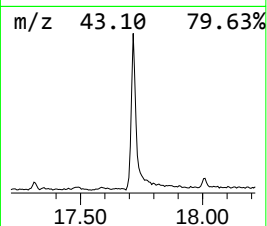
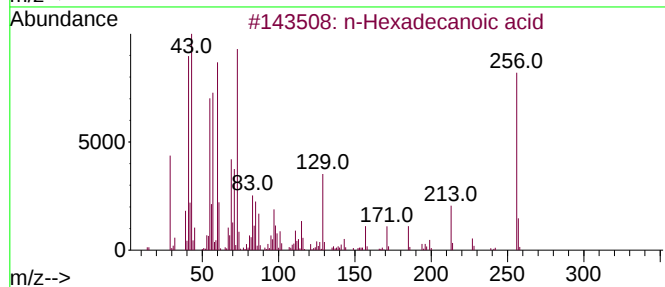
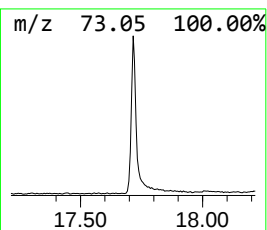
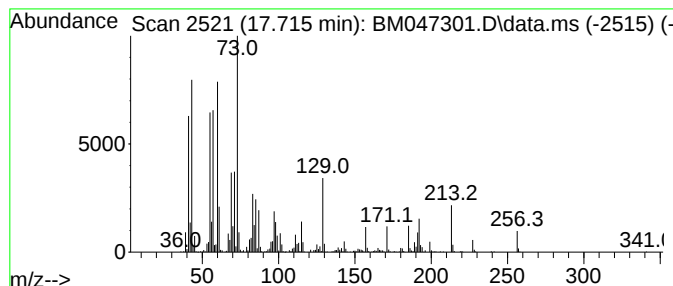
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	8.53 ng	1153720	Phenanthrene-d10	16.780

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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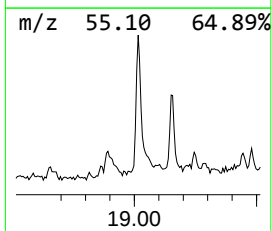
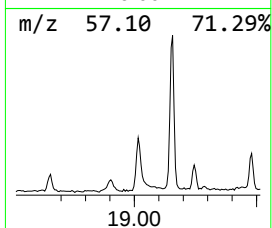
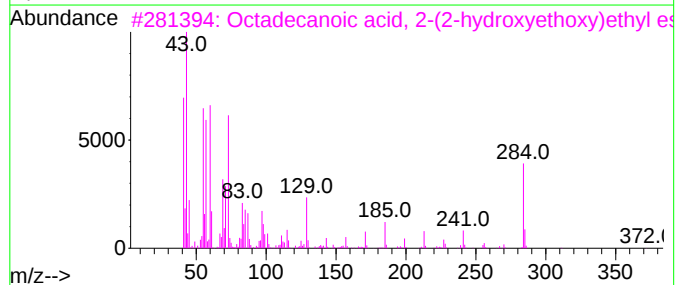
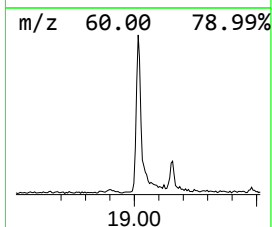
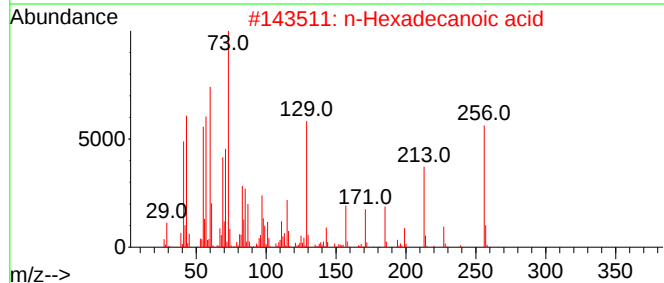
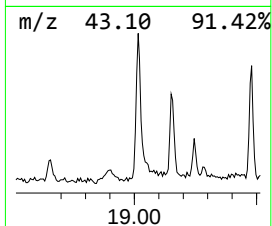
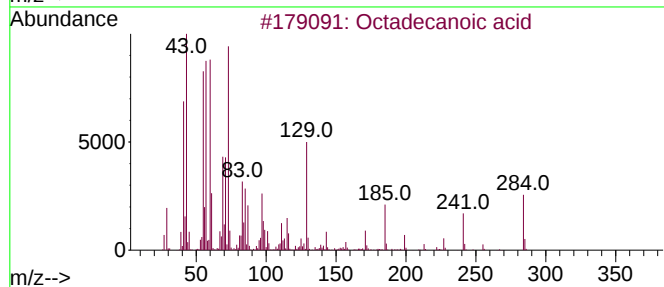
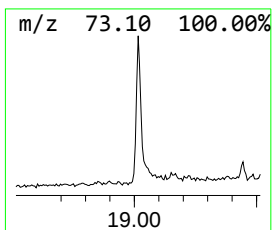
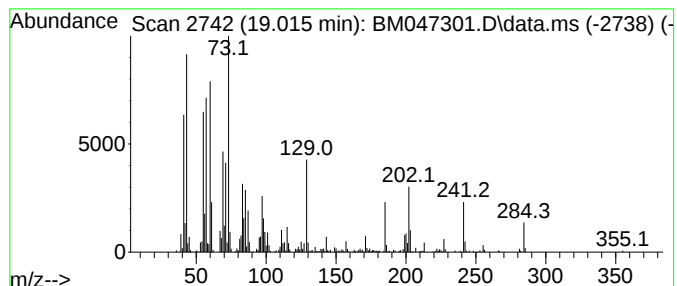
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	2.61 ng	506430	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	74
4			Dodecanoic acid	200	C12H24O2	000143-07-7	70
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047301.D
Acq On : 21 Aug 2024 17:06
Operator : RC/JU
Sample : P3617-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B5-081424-10-14

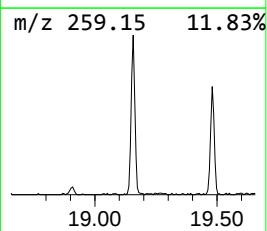
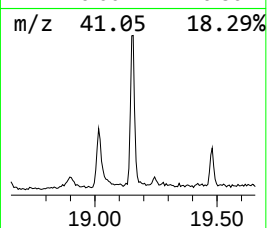
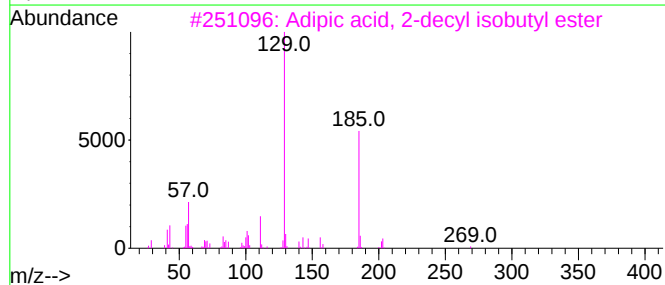
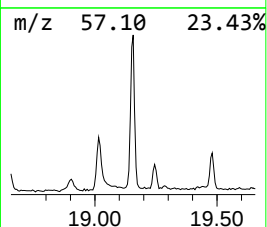
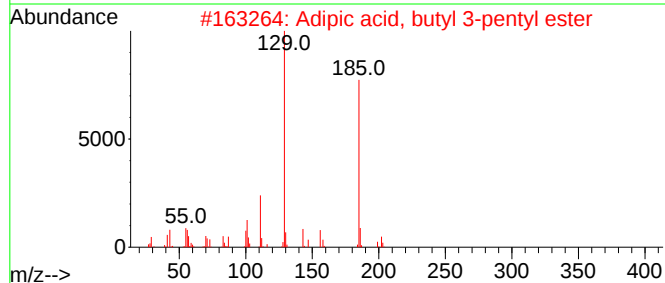
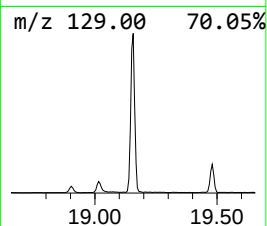
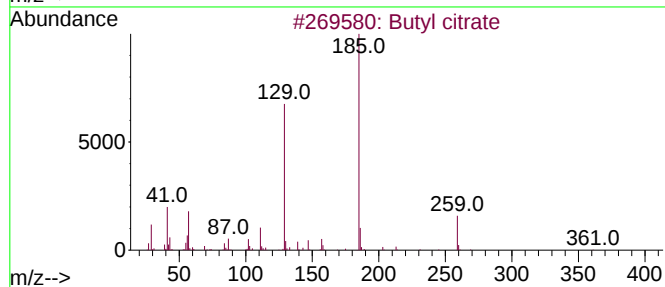
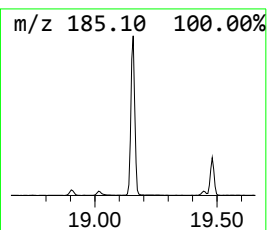
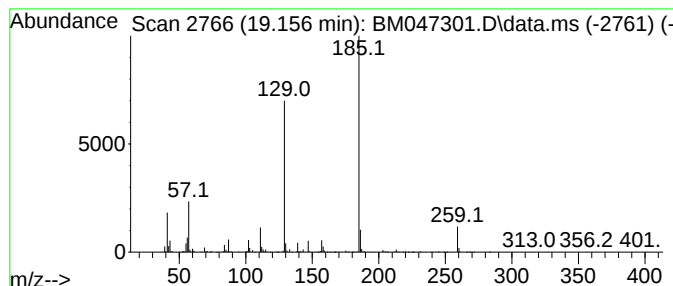
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butyl citrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.157	4.82 ng	936877	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	76
2			Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	72
3			Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	72
4			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	56
5			Adipic acid, 3,3-dimethylbut-2-y...	286	C16H30O4	1000353-66-7	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047301.D
Acq On : 21 Aug 2024 17:06
Operator : RC/JU
Sample : P3617-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VCPS-B5-081424-10-14

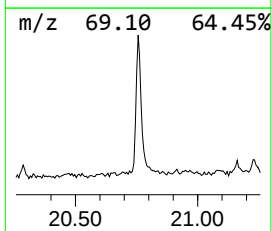
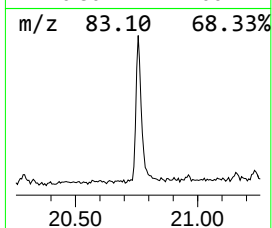
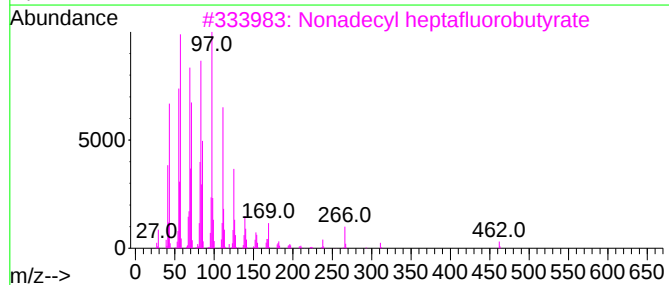
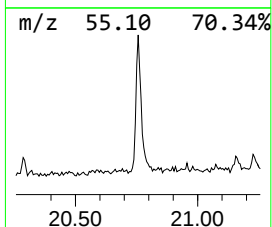
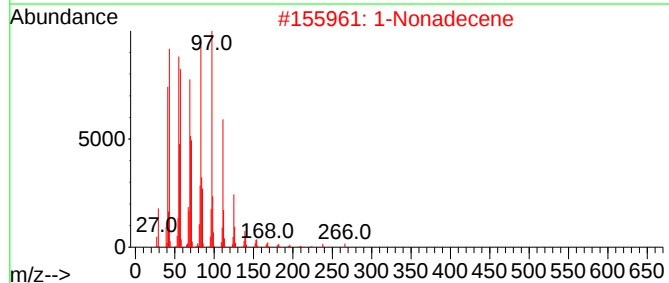
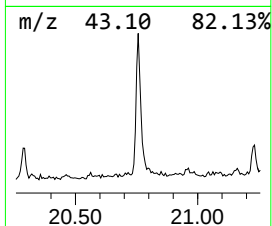
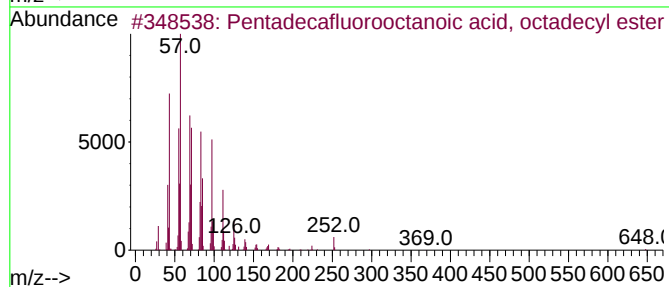
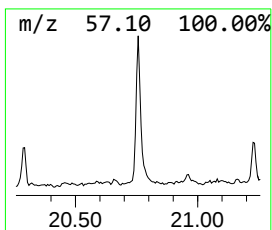
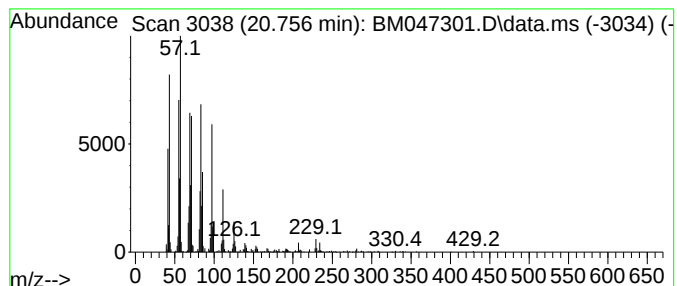
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	4.07 ng	790618	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Nonadecene	266	C19H38	018435-45-5	93
3			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047301.D
Acq On : 21 Aug 2024 17:06
Operator : RC/JU
Sample : P3617-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B5-081424-10-14

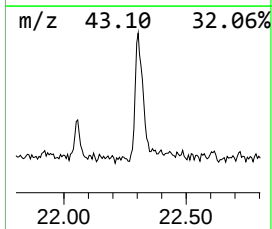
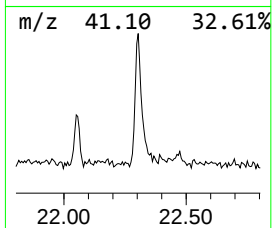
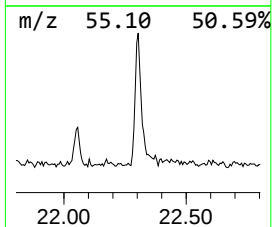
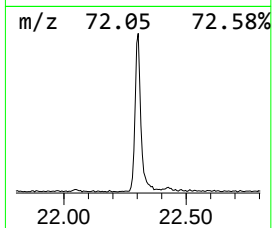
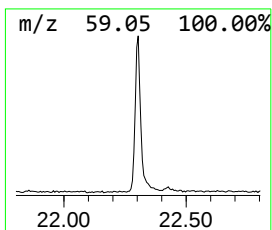
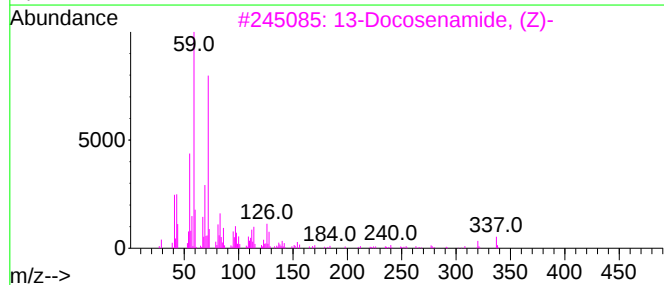
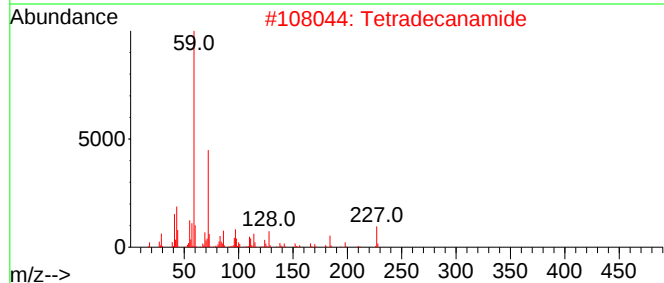
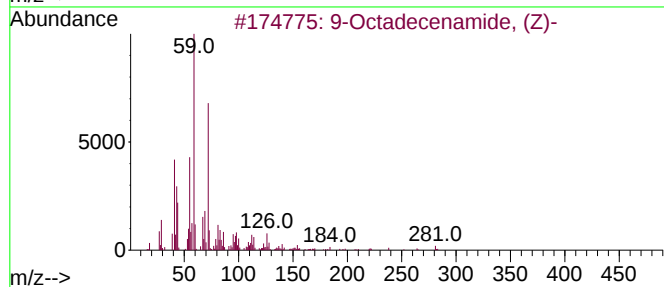
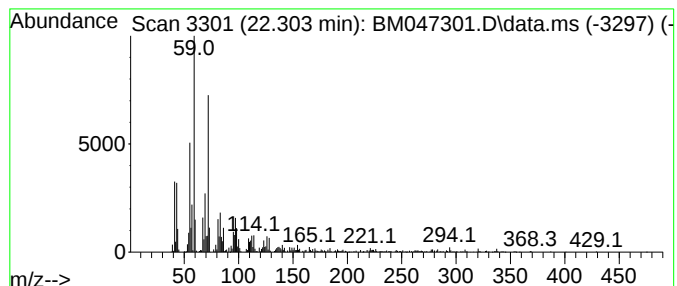
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.303	3.36 ng	652608	Chrysene-d12	21.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			Tetradecanamide	227	C14H29NO	000638-58-4	78
3			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	74
4			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
5			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047301.D
Acq On : 21 Aug 2024 17:06
Operator : RC/JU
Sample : P3617-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
VCPS-B5-081424-10-14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.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
Propylene Glycol	3.257	3.9	ng	229818	1	7.351	1177690	20.0
2-Pentanone, 4-...	4.563	4.3	ng	251553	1	7.351	1177690	20.0
1-Phenoxypropan...	10.875	3.5	ng	274938	2	10.110	1577860	20.0
n-Hexadecanoic ...	17.715	8.5	ng	1153720	4	16.780	2704020	20.0
Octadecanoic acid	19.015	2.6	ng	506430	5	21.015	3884210	20.0
Butyl citrate	19.157	4.8	ng	936877	5	21.015	3884210	20.0
Pentadecafluoro...	20.756	4.1	ng	790618	5	21.015	3884210	20.0
9-Octadecenamid...	22.303	3.4	ng	652608	5	21.015	3884210	20.0