

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
 Data File : BM029264.D
 Acq On : 30 Mar 2021 03:11
 Operator : CG/JU
 Sample : M1828-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FS-SB13(5-6)

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-BM032621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029264.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	17	22	26	rBV	546358	631328	9.60%	1.451%
2	3.058	26	29	35	rVB	104892	122873	1.87%	0.282%
3	4.905	338	343	351	rVB	232618	326045	4.96%	0.750%
4	5.363	414	421	430	rBV	2161242	3043835	46.28%	6.998%
5	6.940	679	689	704	rBV	2153490	3418408	51.97%	7.859%
6	7.757	822	828	835	rVB	563080	869463	13.22%	1.999%
7	8.910	1016	1024	1035	rBV	1371109	2224367	33.82%	5.114%
8	10.539	1293	1301	1308	rBV	732356	1241523	18.87%	2.854%
9	11.569	1471	1476	1483	rBV3	59772	97168	1.48%	0.223%
10	11.969	1537	1544	1550	rBV	79222	129789	1.97%	0.298%
11	12.928	1702	1707	1712	rVB	77336	110649	1.68%	0.254%
12	13.010	1712	1721	1729	rBV	3188348	4700168	71.46%	10.806%
13	13.216	1749	1756	1764	rBV	109438	198511	3.02%	0.456%
14	13.839	1858	1862	1866	rBV	88829	139983	2.13%	0.322%
15	13.875	1866	1868	1872	rVB2	76467	95414	1.45%	0.219%
16	14.292	1934	1939	1947	rVB	70847	99653	1.52%	0.229%
17	14.386	1947	1955	1962	rBV	1045780	1591868	24.20%	3.660%
18	15.869	2201	2207	2214	rBV	1995928	2858636	43.46%	6.572%
19	17.121	2414	2420	2425	rBV	1284677	1799050	27.35%	4.136%
20	17.163	2425	2427	2432	rVB	151909	172047	2.62%	0.396%
21	17.251	2438	2442	2446	rVB	65214	92762	1.41%	0.213%
22	18.021	2566	2573	2583	rBV2	550655	859393	13.07%	1.976%
23	19.180	2762	2770	2783	rBV2	1189046	2706368	41.14%	6.222%
24	19.298	2787	2790	2799	rVB2	283152	510423	7.76%	1.173%
25	19.457	2813	2817	2821	rVB	140120	176330	2.68%	0.405%
26	19.504	2822	2825	2826	rVV	66224	69382	1.05%	0.160%
27	19.539	2826	2831	2838	rVB	524152	766117	11.65%	1.761%
28	19.745	2860	2866	2871	rBV	5454687	6577649	100.00%	15.122%
29	20.433	2979	2983	2994	rBV	546248	854089	12.98%	1.964%
30	20.539	2998	3001	3007	rVB	189023	234481	3.56%	0.539%
31	21.009	3077	3081	3088	rVB3	740203	920393	13.99%	2.116%
32	21.209	3113	3115	3119	rVB	146817	141308	2.15%	0.325%
33	21.292	3122	3129	3133	rBV2	1713877	2617359	39.79%	6.017%
34	22.139	3270	3273	3278	rVB	311729	372045	5.66%	0.855%
35	22.339	3303	3307	3313	rBV2	361810	582286	8.85%	1.339%
36	22.856	3392	3395	3400	rBV	205537	290468	4.42%	0.668%

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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-BM032621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.527	3504	3509	3515	rBV2	1004736	1855554	28.21%	4.266%
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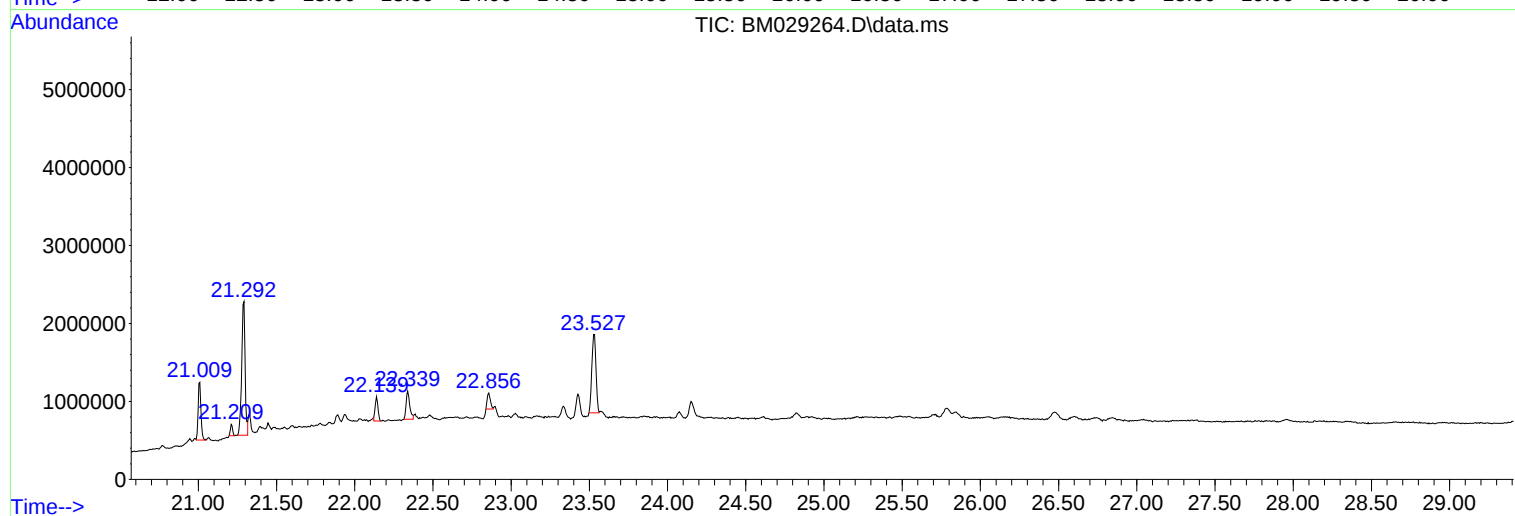
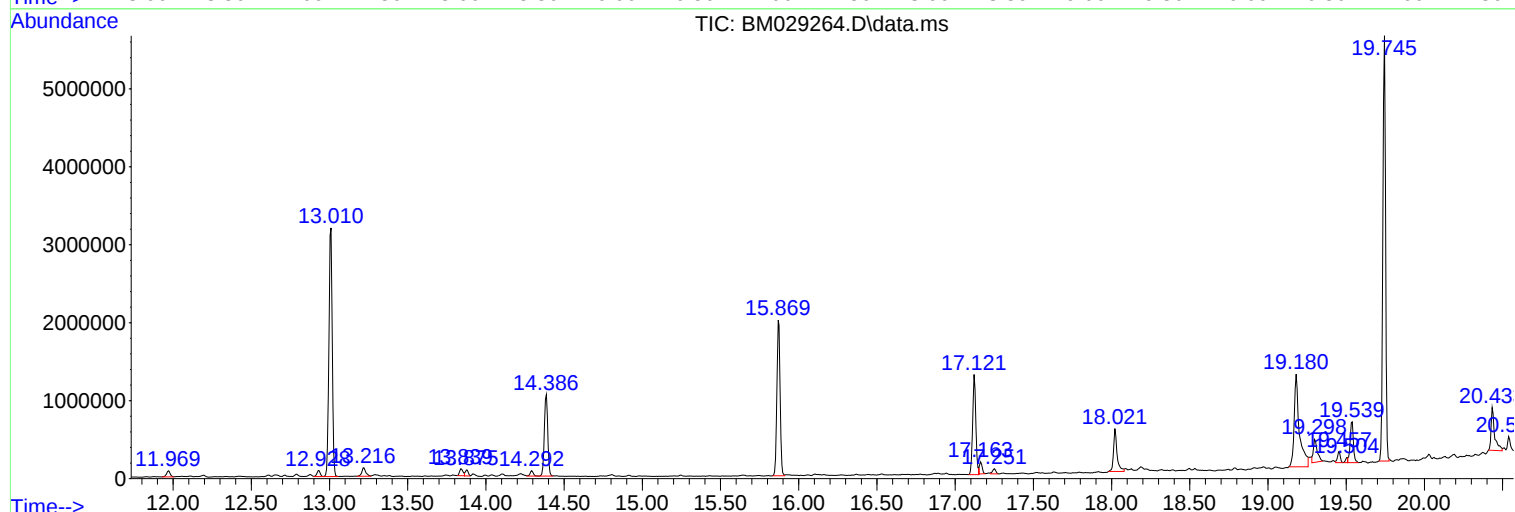
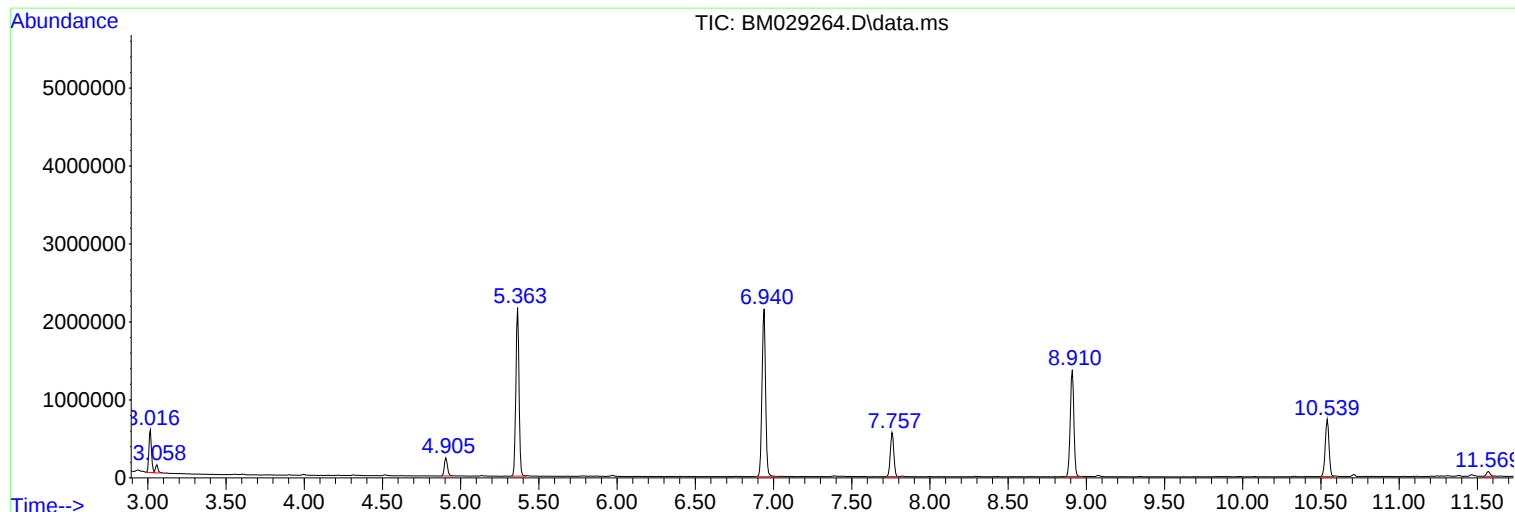
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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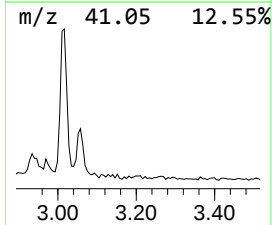
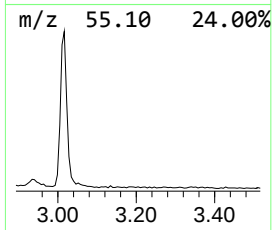
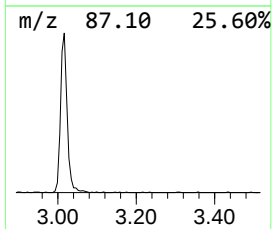
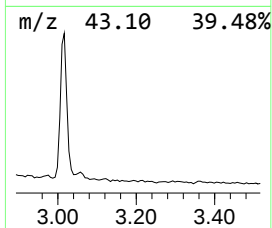
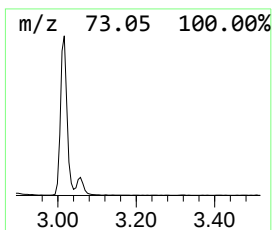
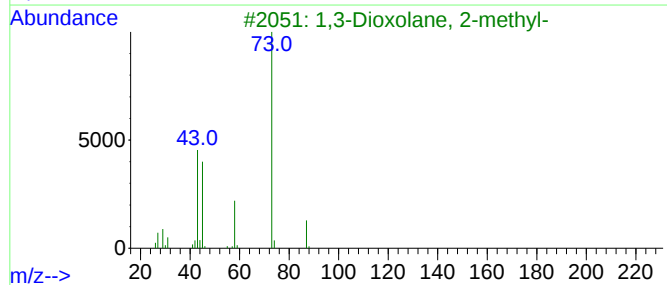
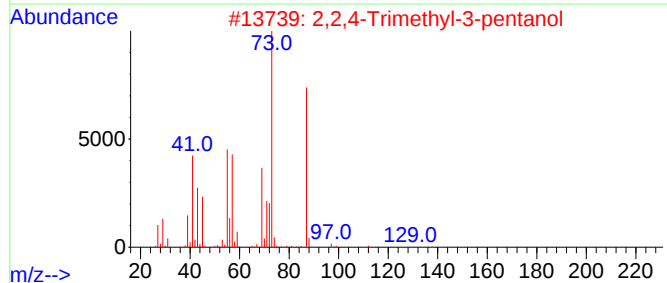
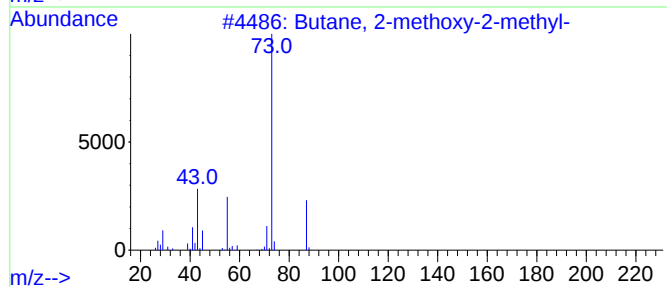
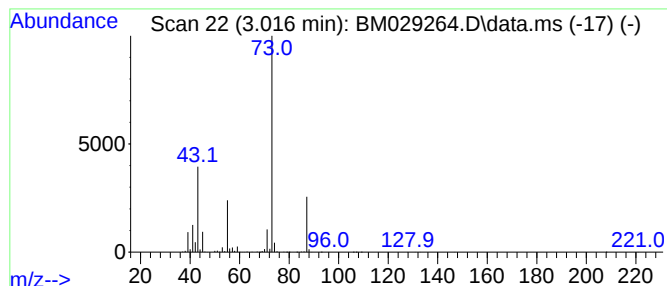
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
3.016	14.52 ng	631328	1,4-Dichlorobenzene-d4	7.757

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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Instrument :
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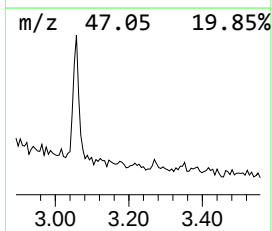
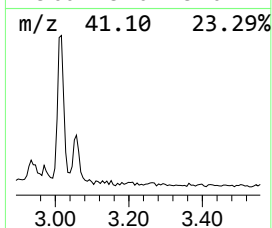
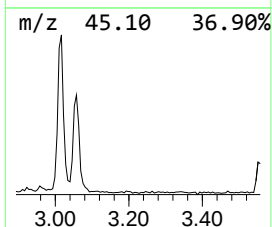
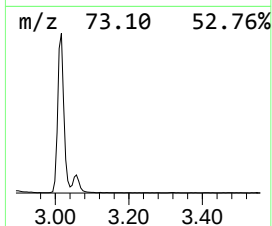
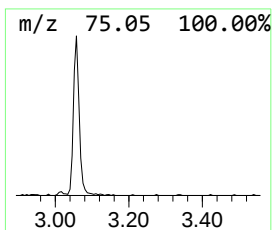
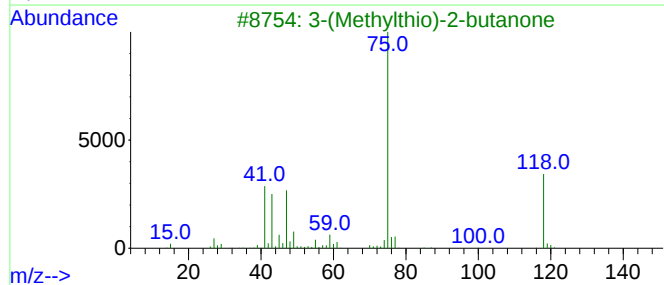
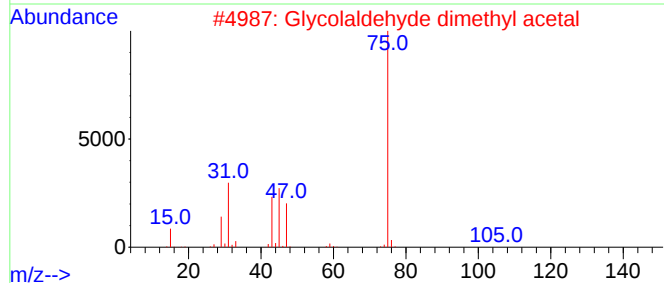
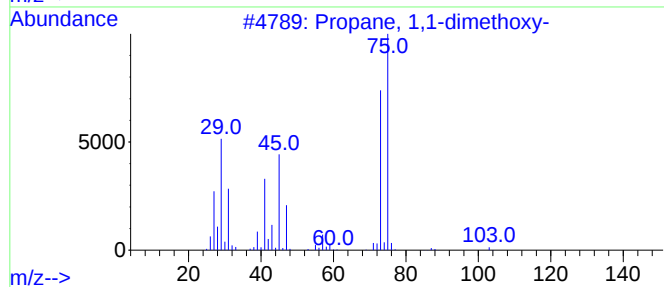
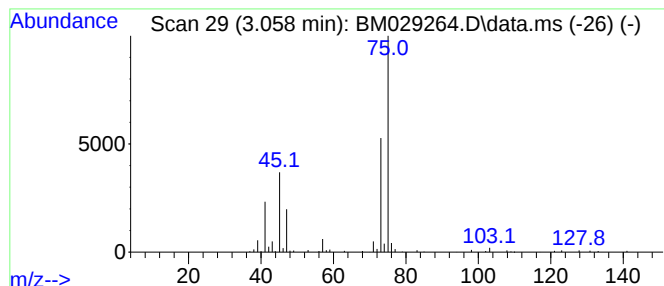
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.058	2.83 ng	122873	1,4-Dichlorobenzene-d4	7.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	56
3			3-(Methylthio)-2-butanone	118	C5H10OS	053475-15-3	45
4			2-Propanol, 1,1-dimethoxy-, acetate	162	C7H14O4	074495-37-7	45
5			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	39



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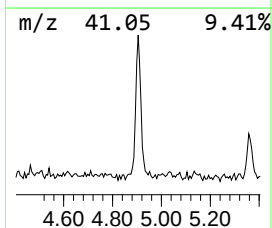
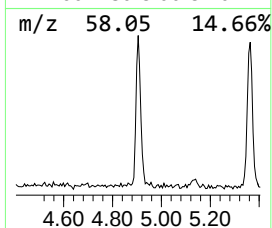
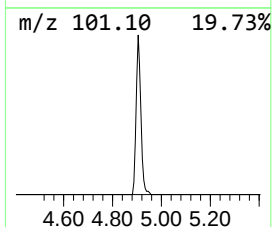
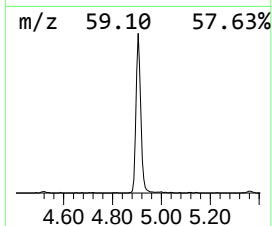
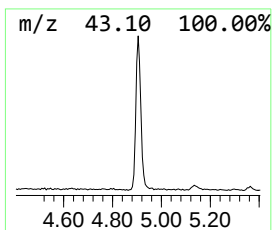
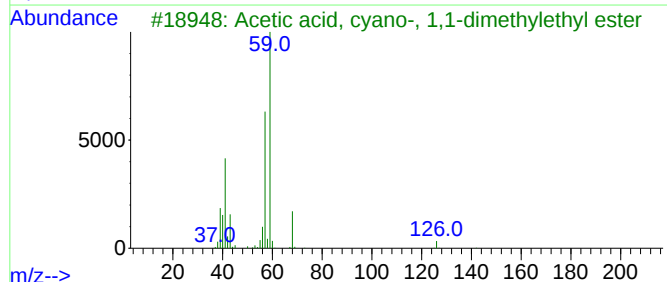
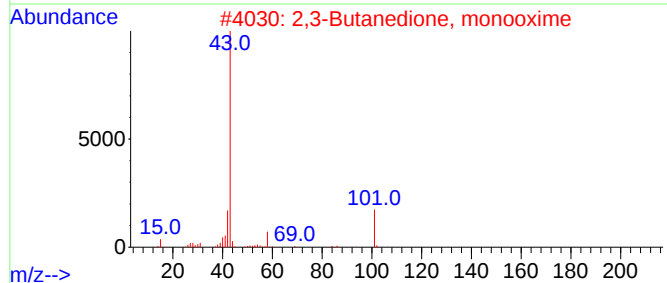
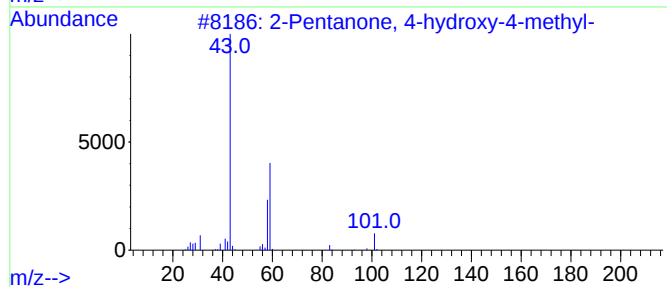
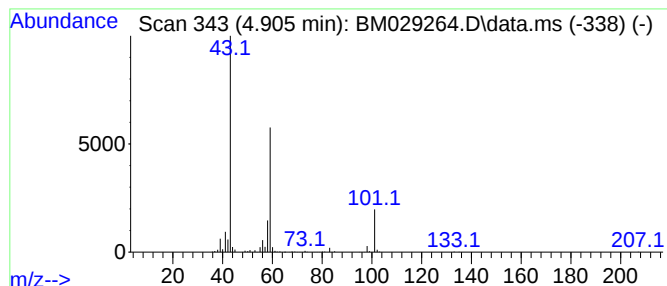
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	7.50 ng	326045	1,4-Dichlorobenzene-d4	7.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Butane	58	C4H10	000106-97-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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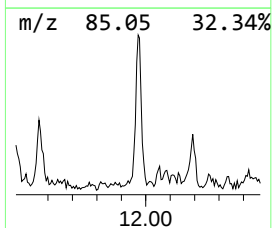
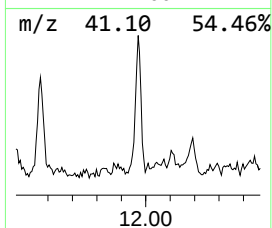
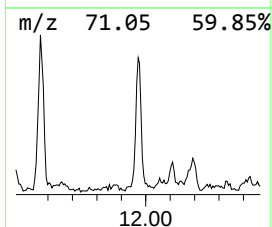
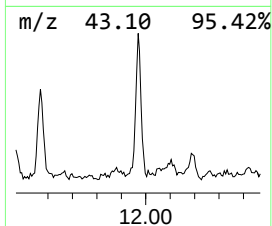
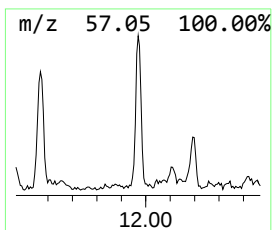
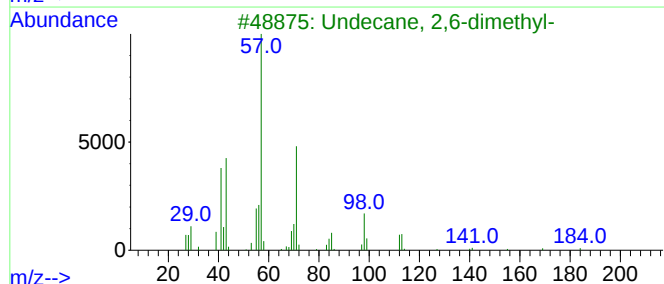
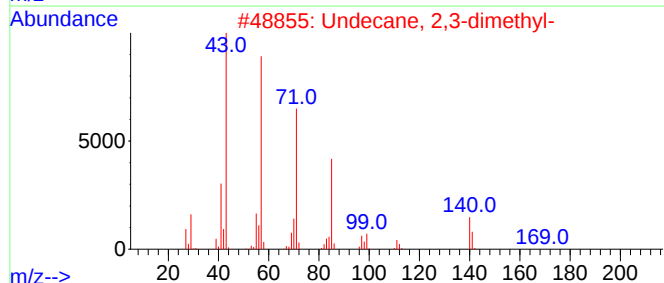
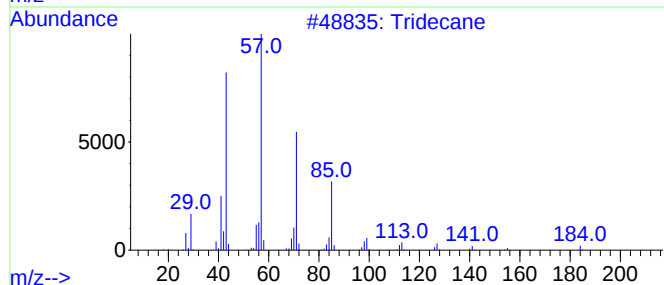
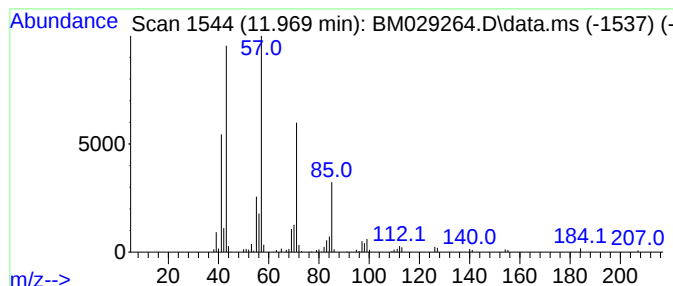
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.09 ng	129789	Naphthalene-d8	10.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	90
2			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	86
3			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	81
4			Tetradecane	198	C14H30	000629-59-4	80
5			Heneicosane	296	C21H44	000629-94-7	78



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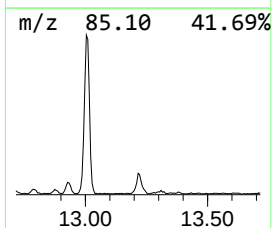
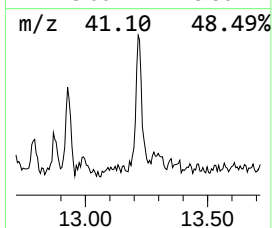
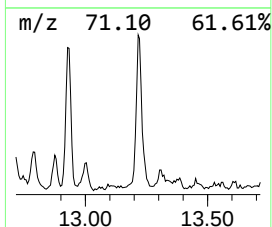
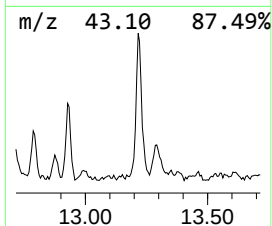
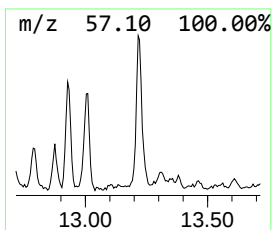
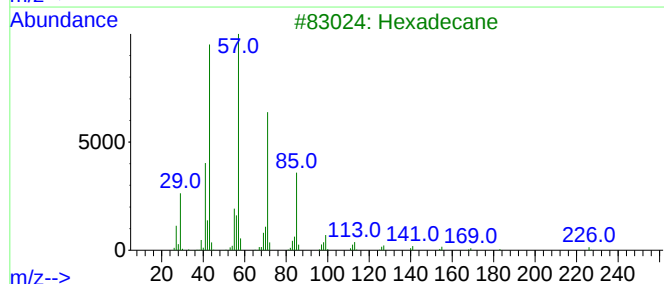
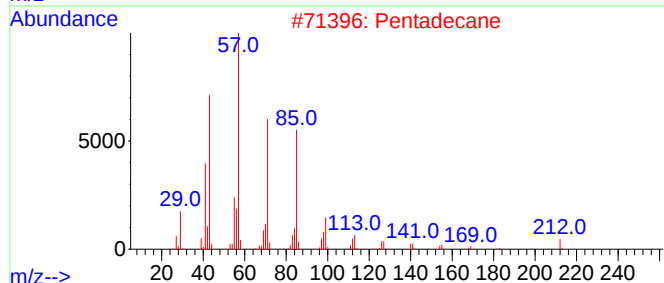
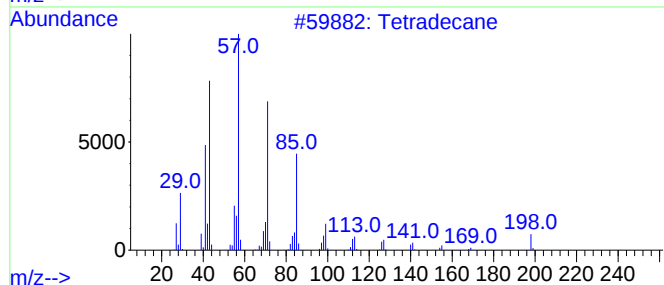
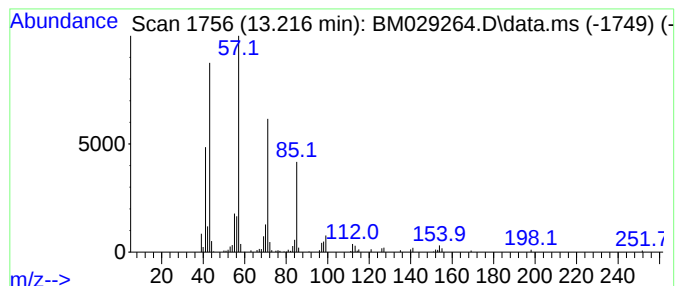
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	2.49 ng	198511	Acenaphthene-d10	14.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	90
2			Pentadecane	212	C15H32	000629-62-9	90
3			Hexadecane	226	C16H34	000544-76-3	87
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5			Tridecane	184	C13H28	000629-50-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029264.D
Acq On : 30 Mar 2021 03:11
Operator : CG/JU
Sample : M1828-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB13(5-6)

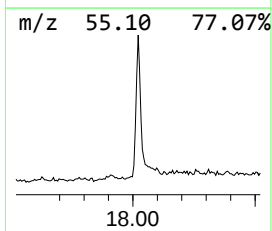
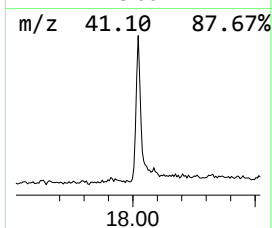
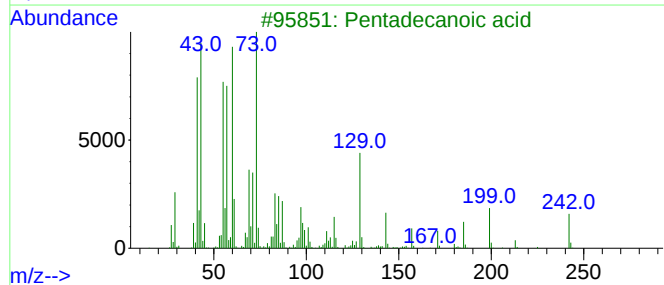
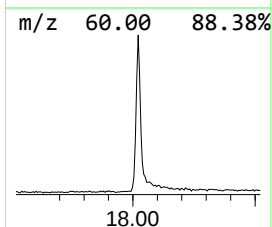
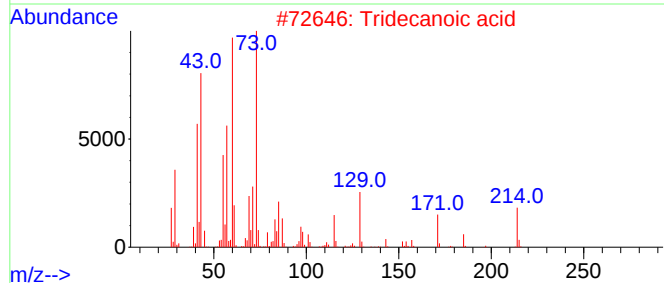
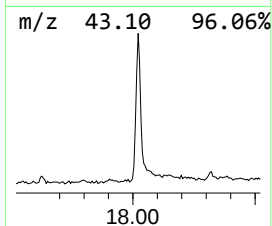
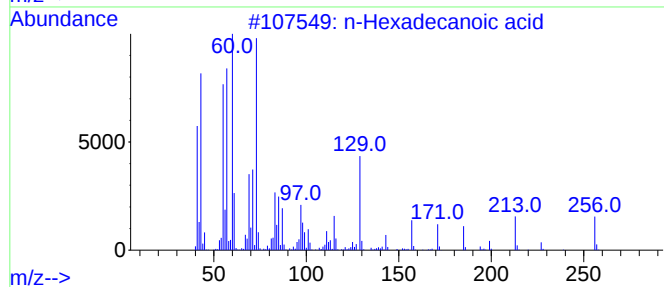
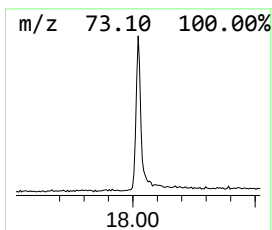
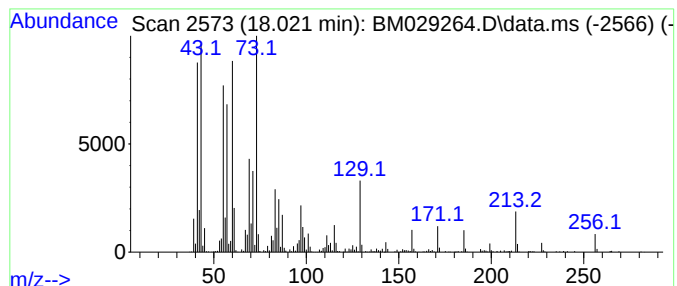
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.021	9.55 ng	859393	Phenanthrene-d10	17.121

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029264.D
Acq On : 30 Mar 2021 03:11
Operator : CG/JU
Sample : M1828-01
Misc :
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Instrument :
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ClientSampleId :
FS-SB13(5-6)

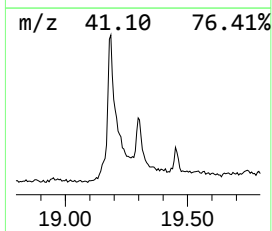
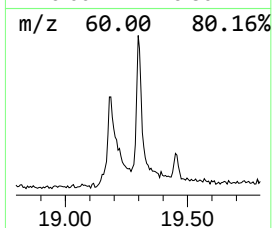
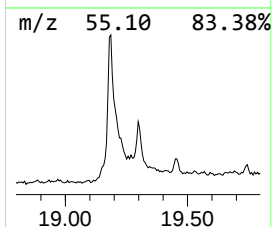
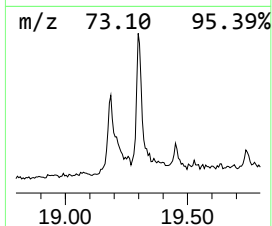
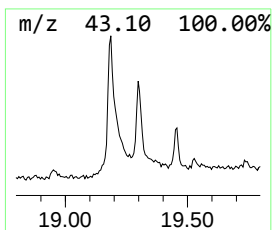
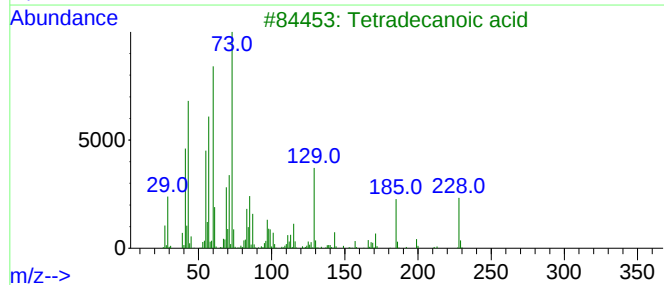
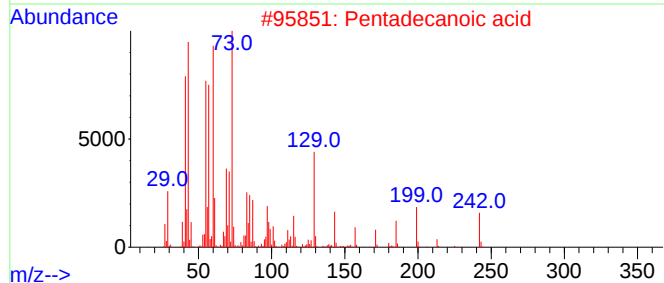
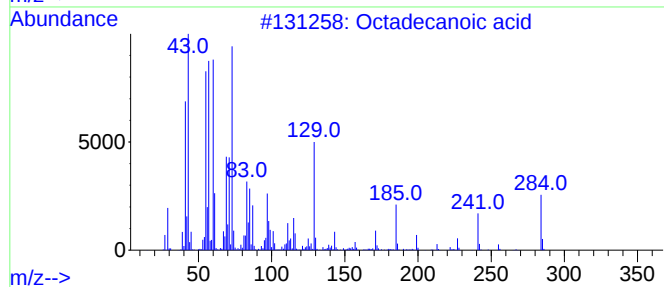
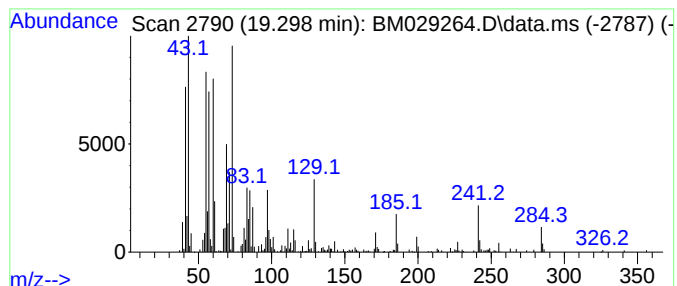
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.298	3.90 ng	510423	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029264.D
Acq On : 30 Mar 2021 03:11
Operator : CG/JU
Sample : M1828-01
Misc :
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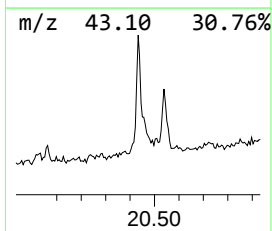
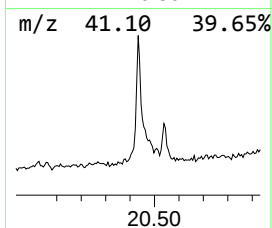
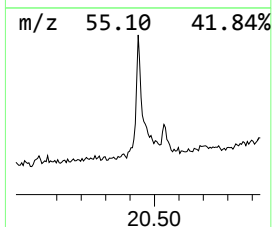
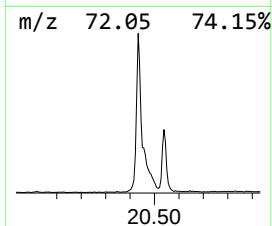
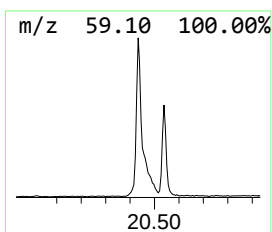
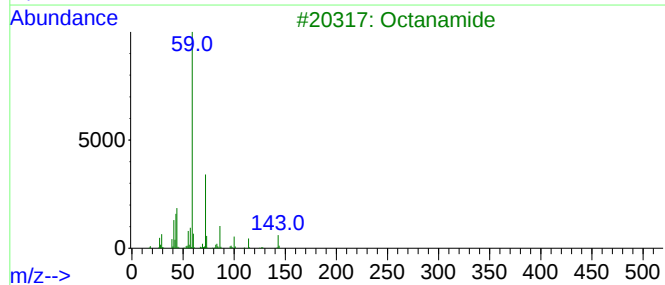
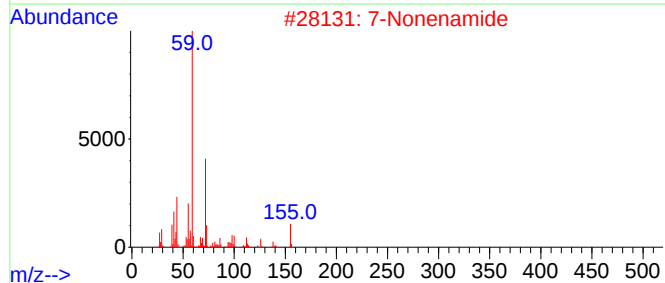
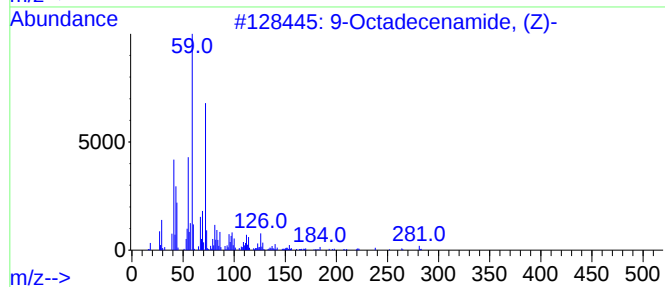
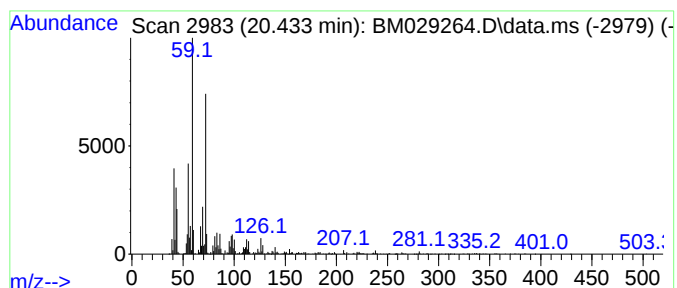
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ClientSampleId :
FS-SB13(5-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.433	6.53 ng	854089	Chrysene-d12	21.292	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	7-Nonenamide	155	C9H17NO	090949-53-4	50
3	Octanamide	143	C8H17NO	000629-01-6	50
4	Dodecanamide	199	C12H25NO	001120-16-7	47
5	Nonanamide	157	C9H19NO	001120-07-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029264.D
Acq On : 30 Mar 2021 03:11
Operator : CG/JU
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Instrument :
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ClientSampleId :
FS-SB13(5-6)

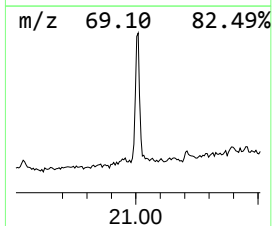
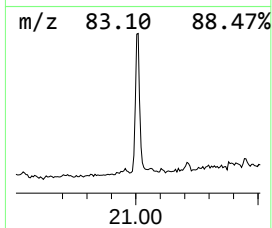
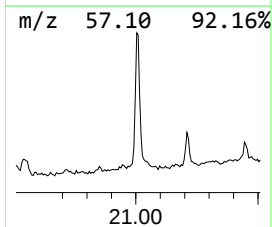
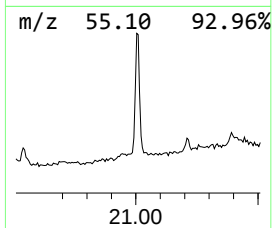
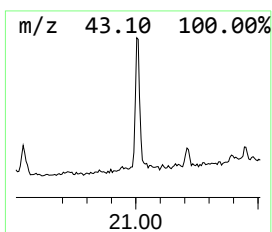
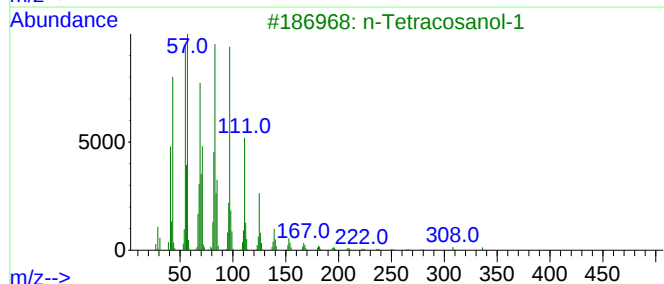
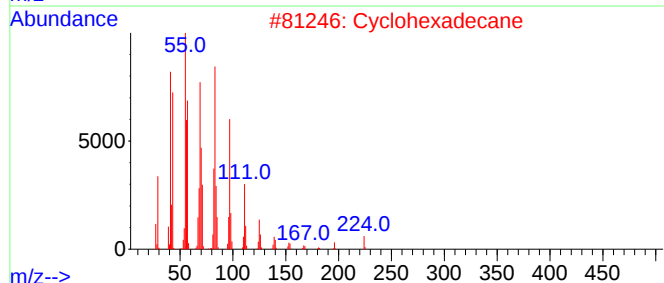
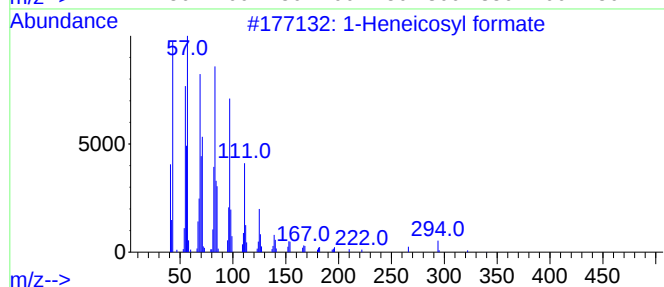
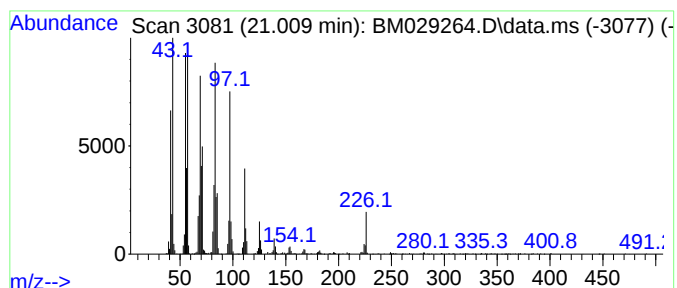
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.009	7.03 ng	920393	Chrysene-d12	21.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2		Cyclohexadecane	224	C16H32	000295-65-8	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029264.D
Acq On : 30 Mar 2021 03:11
Operator : CG/JU
Sample : M1828-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FS-SB13(5-6)

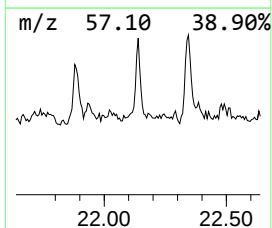
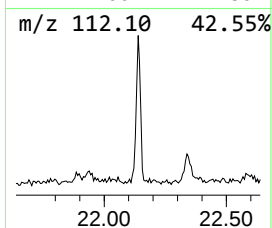
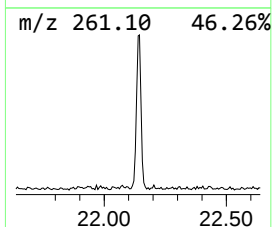
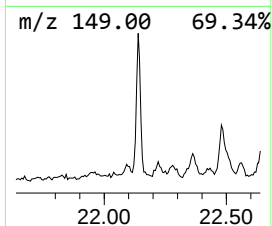
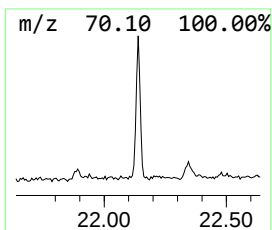
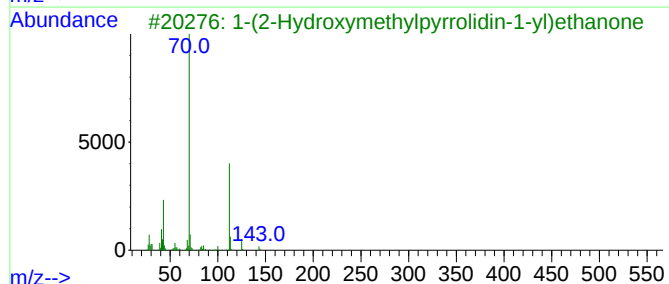
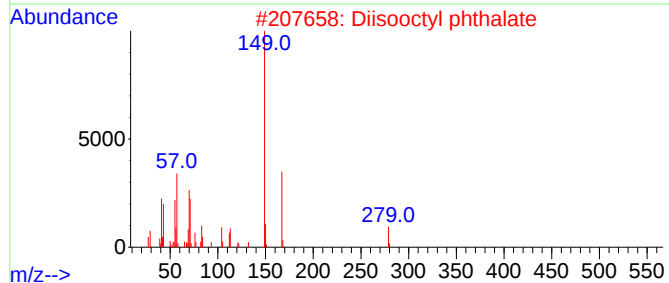
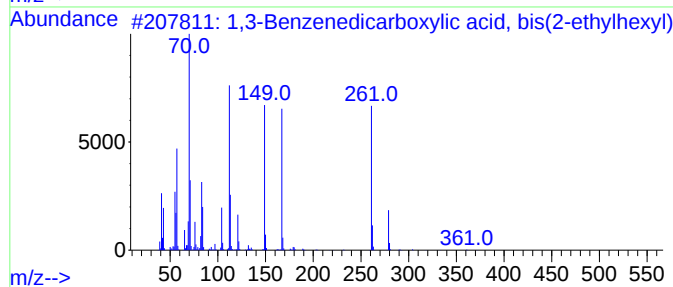
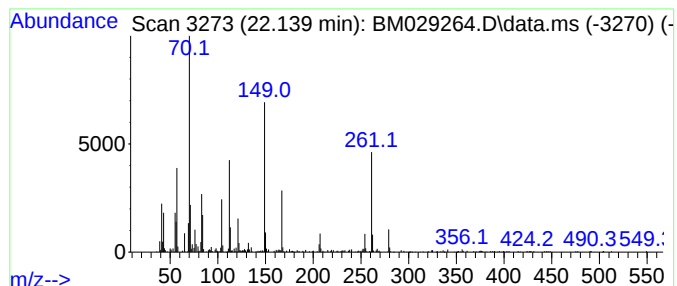
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown22.139 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.139	2.84 ng	372045	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	35
2			Diisooctyl phthalate	390	C24H38O4	000131-20-4	25
3			1-(2-Hydroxymethylpyrrolidin-1-y...	143	C7H13NO2	1000192-83-2	25
4			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	25
5			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029264.D
Acq On : 30 Mar 2021 03:11
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ClientSampleId :
FS-SB13(5-6)

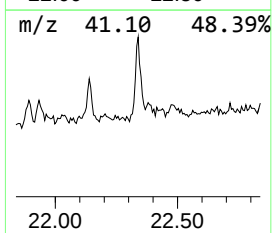
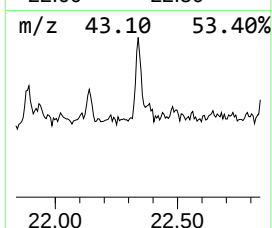
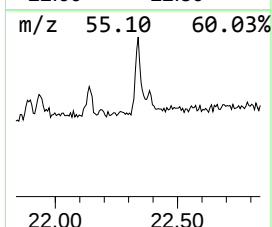
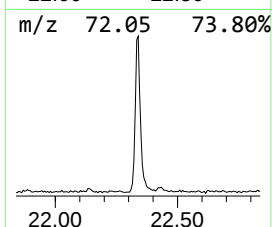
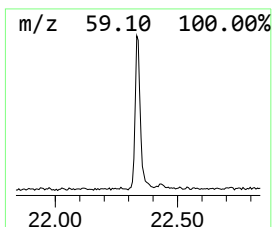
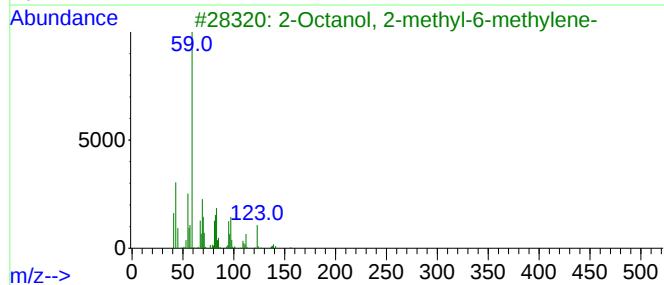
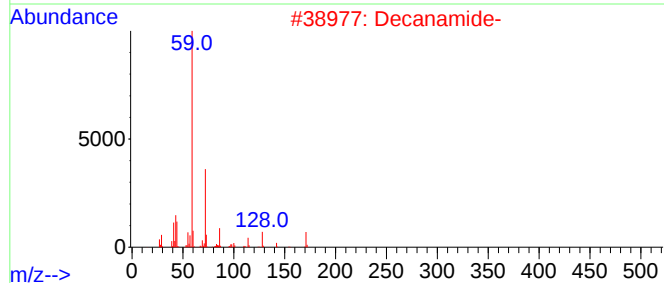
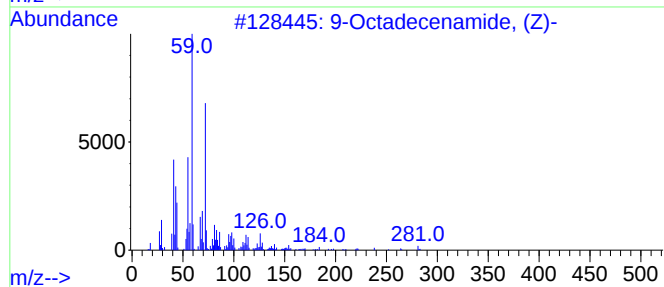
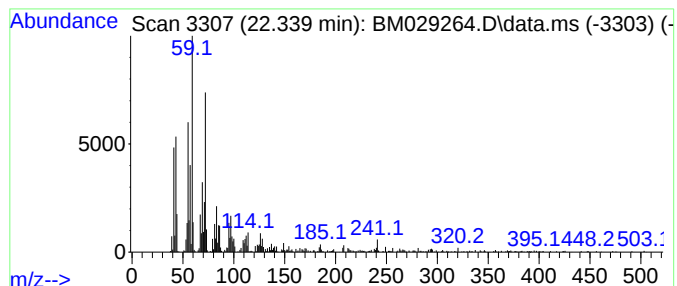
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Decanamide- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.339	4.45 ng	582286	Chrysene-d12	21.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		Decanamide-	171	C10H21NO	002319-29-1	59
3		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	50
4		Tetradecanamide	227	C14H29NO	000638-58-4	43
5		3-Hexadecanol	242	C16H34O	000593-03-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032921\
Data File : BM029264.D
Acq On : 30 Mar 2021 03:11
Operator : CG/JU
Sample : M1828-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB13(5-6)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Propane, 1,1-di...	3.058	2.8	ng	122873	1	7.757	869463	20.0
2-Pentanone, 4-...	4.905	7.5	ng	326045	1	7.757	869463	20.0
Tridecane	11.969	2.1	ng	129789	2	10.540	1241520	20.0
Tetradecane	13.216	2.5	ng	198511	3	14.386	1591870	20.0
n-Hexadecanoic ...	18.021	9.6	ng	859393	4	17.121	1799050	20.0
Octadecanoic acid	19.298	3.9	ng	510423	5	21.292	2617360	20.0
9-Octadecenamid...	20.433	6.5	ng	854089	5	21.292	2617360	20.0
1-Heneicosyl fo...	21.009	7.0	ng	920393	5	21.292	2617360	20.0
unknown22.139	22.139	2.8	ng	372045	5	21.292	2617360	20.0
Decanamide-	22.339	4.5	ng	582286	5	21.292	2617360	20.0