

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
 Data File : BM049804.D
 Acq On : 03 Apr 2025 13:58
 Operator : RC/JU
 Sample : Q1693-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WCS-TP-3

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-BM031325.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049804.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	3	5	16	rVB	124097	174695	1.40%	0.248%
2	4.905	320	326	335	rVB	863022	1158820	9.30%	1.646%
3	5.369	399	405	421	rVB	4503601	6120588	49.13%	8.696%
4	5.981	504	509	516	rVB	136976	196800	1.58%	0.280%
5	6.957	667	675	687	rBV	4216994	6240764	50.09%	8.867%
6	7.787	810	816	824	rVB	1032847	1548211	12.43%	2.200%
7	8.940	1003	1012	1023	rBV	2355940	3716756	29.83%	5.281%
8	10.581	1284	1291	1299	rBV	1182822	1894967	15.21%	2.692%
9	13.051	1704	1711	1718	rBV	6225712	8575685	68.83%	12.184%
10	14.427	1935	1945	1952	rBV	1764487	2531911	20.32%	3.597%
11	15.786	2171	2176	2182	rVB	470395	620828	4.98%	0.882%
12	15.916	2191	2198	2207	rBV	5185313	6883281	55.25%	9.780%
13	16.574	2302	2310	2318	rVB6	95793	197567	1.59%	0.281%
14	17.168	2404	2411	2424	rBV	2122391	2904260	23.31%	4.126%
15	18.074	2559	2565	2594	rBV	2497312	3759069	30.17%	5.341%
16	18.339	2606	2610	2614	rBV2	101834	155816	1.25%	0.221%
17	18.392	2615	2619	2626	rVB2	150556	254858	2.05%	0.362%
18	19.227	2758	2761	2771	rVB6	75083	132349	1.06%	0.188%
19	19.351	2777	2782	2794	rBV	1060698	1631771	13.10%	2.318%
20	19.457	2796	2800	2805	rVB	148533	236434	1.90%	0.336%
21	19.792	2852	2857	2863	rBV	11070836	12459035	100.00%	17.702%
22	20.256	2931	2936	2943	rBV2	183183	340749	2.73%	0.484%
23	20.956	3050	3055	3063	rVB	270584	446855	3.59%	0.635%
24	21.092	3074	3078	3089	rBV2	302041	463857	3.72%	0.659%
25	21.403	3125	3131	3137	rBV	2273188	3160162	25.36%	4.490%
26	21.609	3163	3166	3171	rVB2	116454	140609	1.13%	0.200%
27	21.674	3173	3177	3190	rVB	281200	468429	3.76%	0.666%
28	22.497	3313	3317	3328	rVB2	201815	448954	3.60%	0.638%
29	23.003	3399	3403	3409	rVB2	176833	297049	2.38%	0.422%
30	24.403	3633	3641	3656	rVB	1297304	3222333	25.86%	4.578%

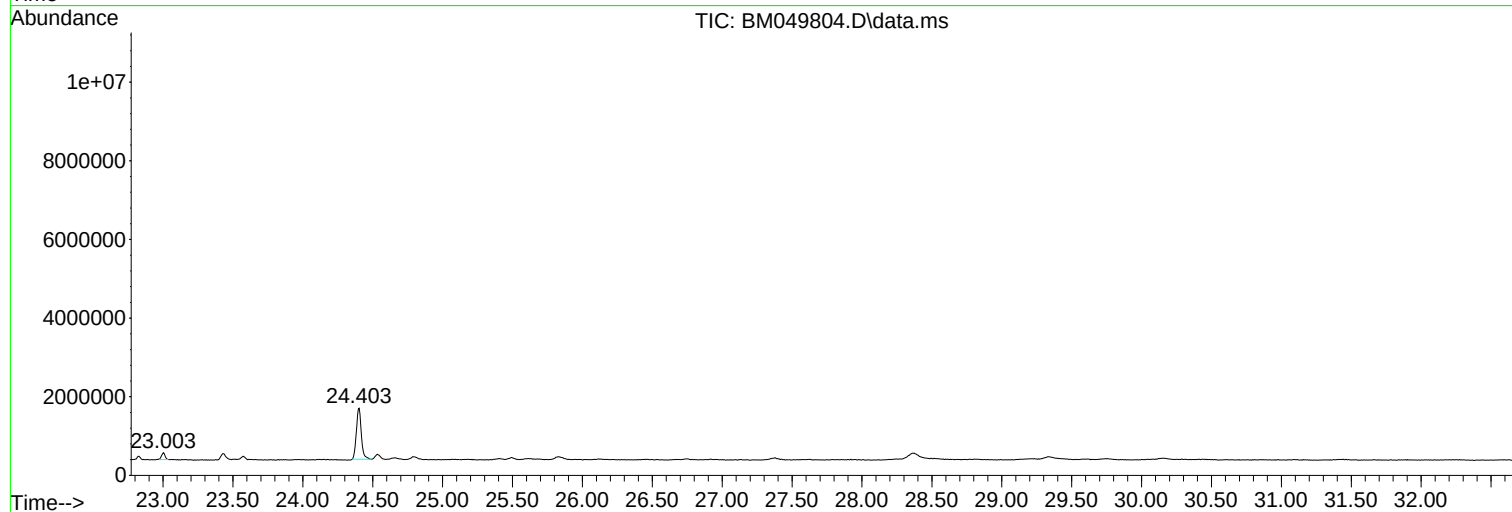
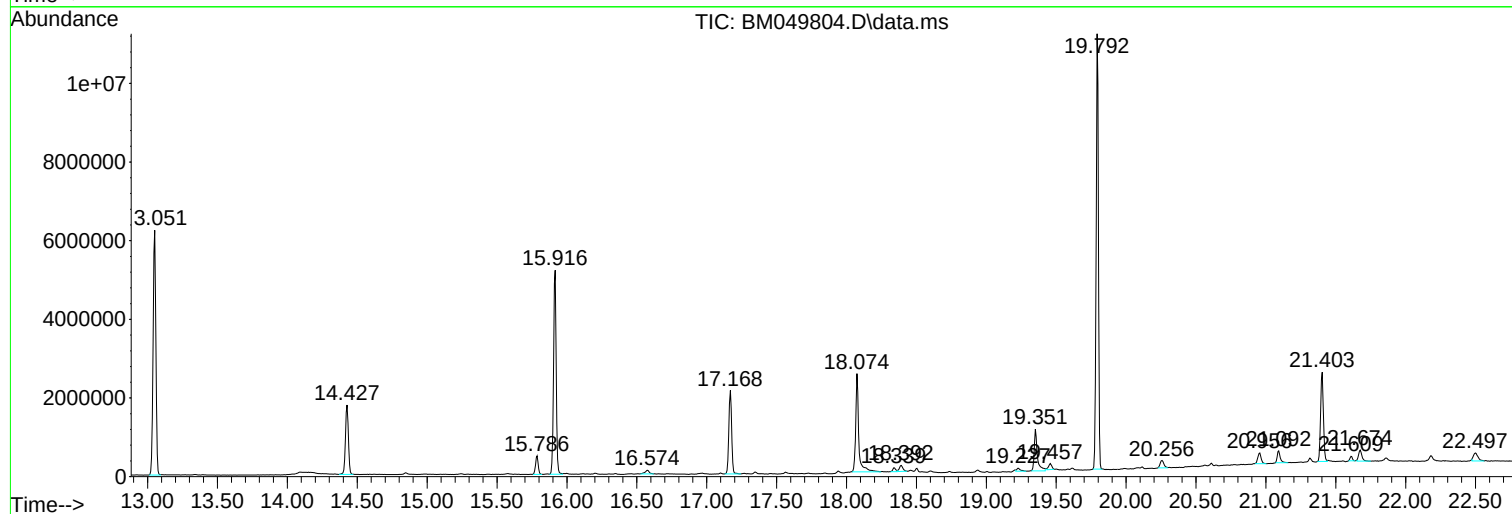
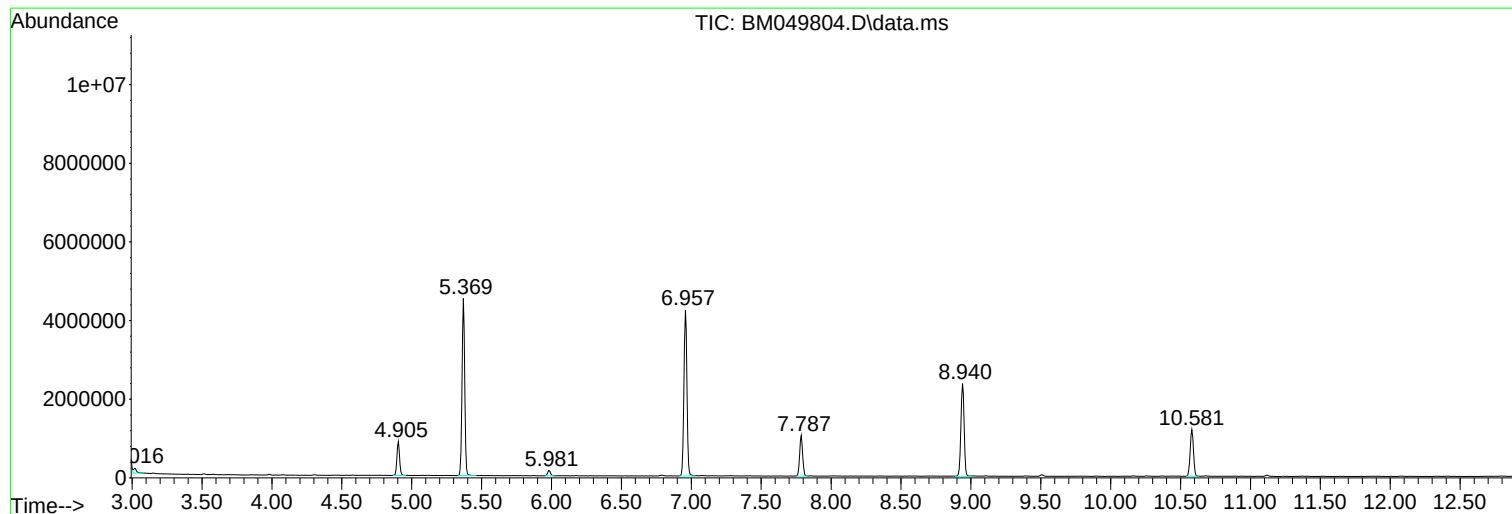
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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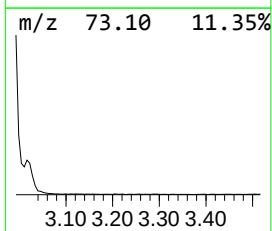
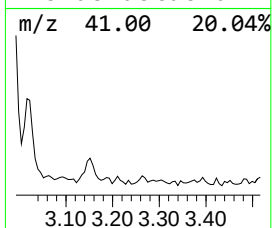
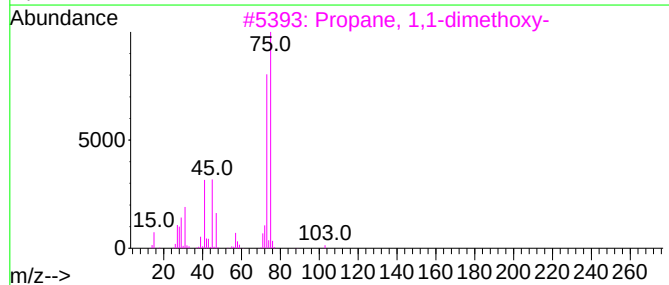
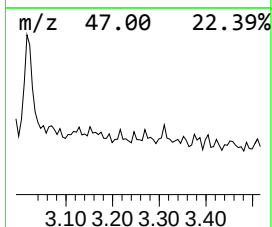
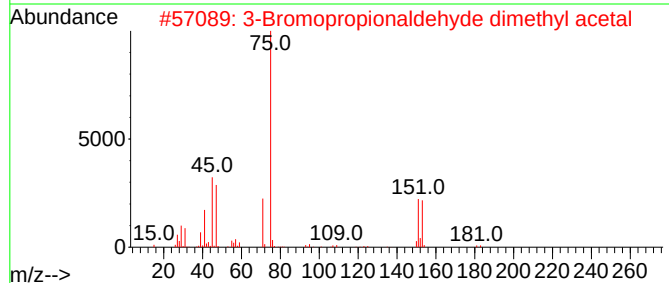
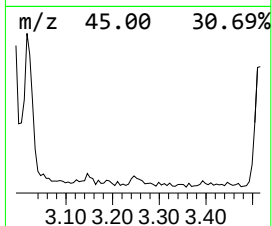
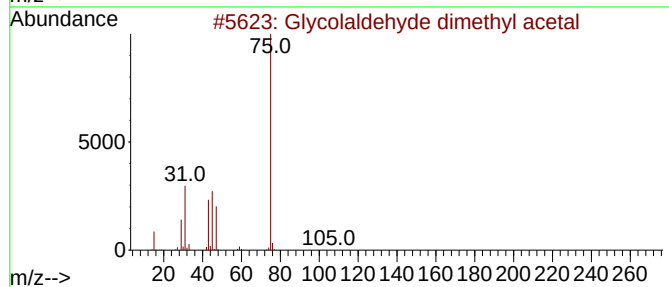
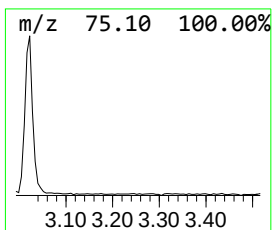
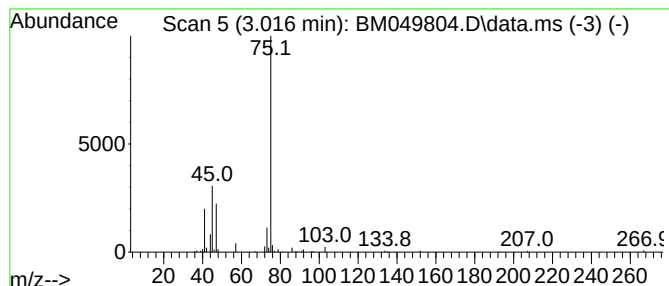
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Glycolaldehyde dimethyl acetal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.016	2.26 ng	174695	1,4-Dichlorobenzene-d4	7.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	72
2			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	72
3			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	40
4			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9
5			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9



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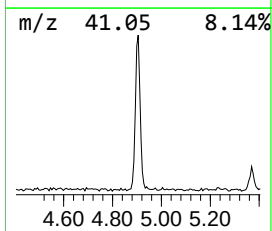
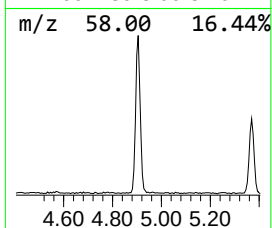
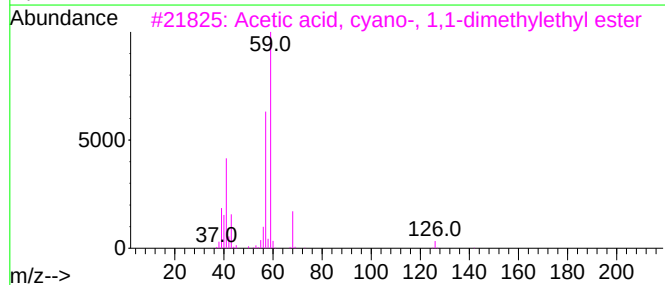
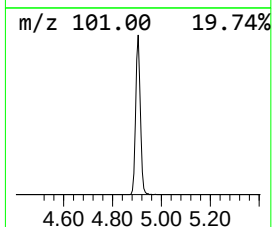
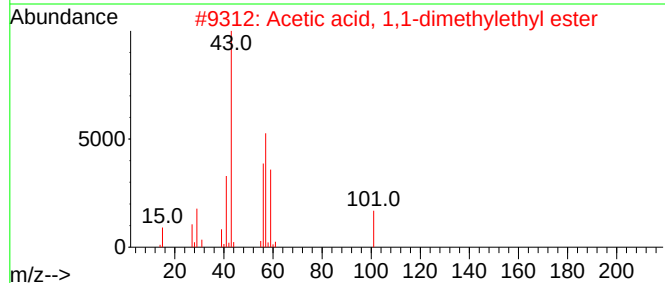
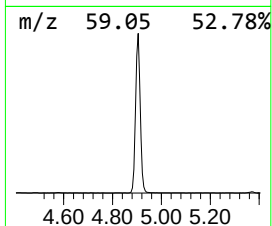
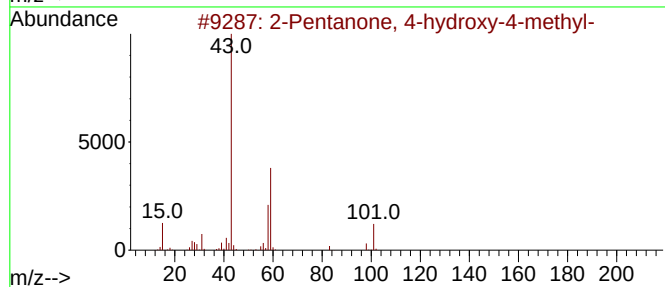
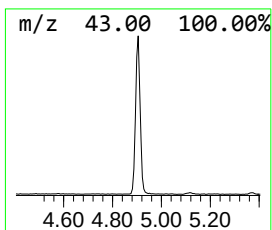
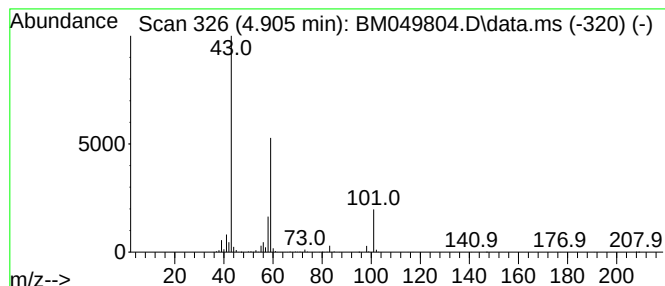
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.905	14.97 ng	1158820	1,4-Dichlorobenzene-d4	7.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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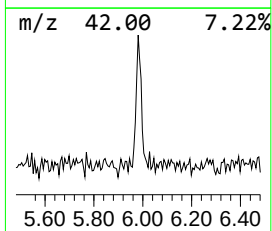
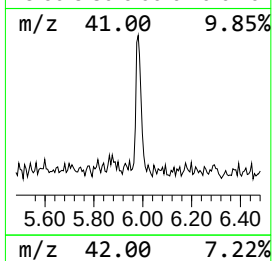
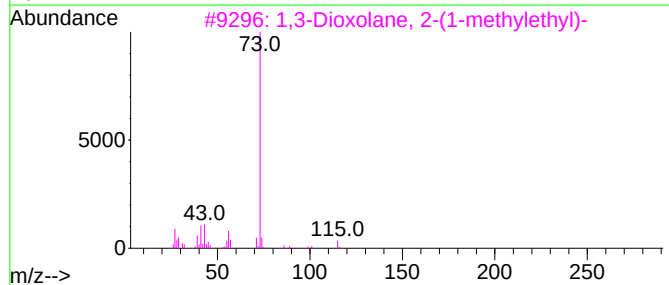
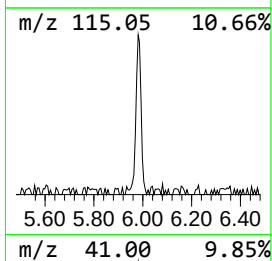
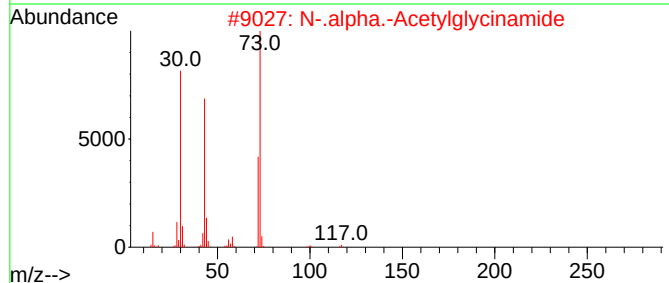
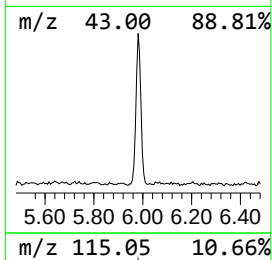
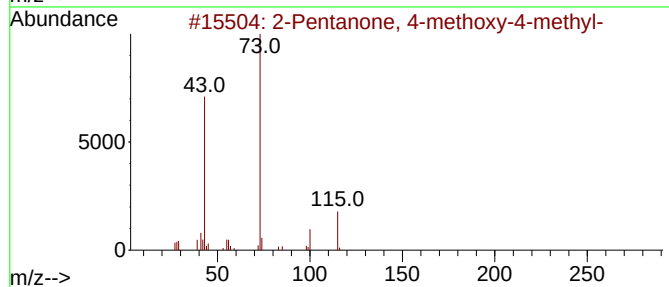
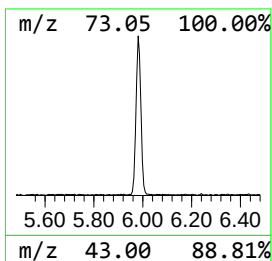
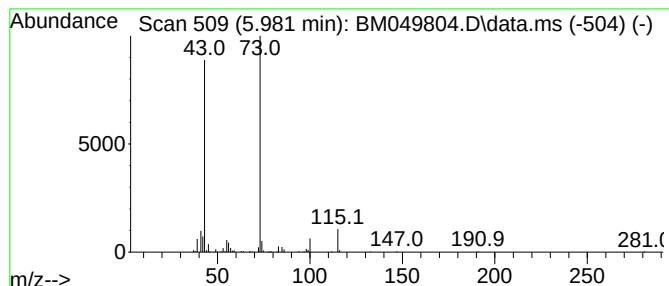
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.981	2.54 ng	196800	1,4-Dichlorobenzene-d4	7.787

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	25
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	14
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9
5		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9



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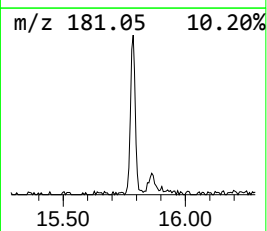
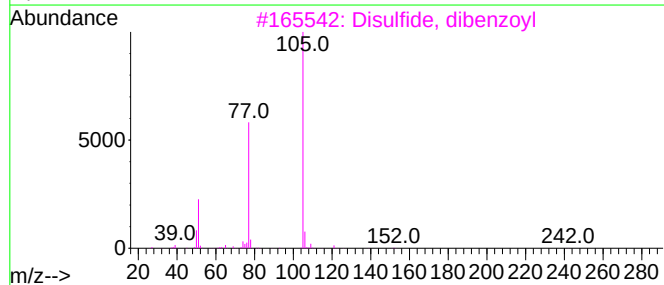
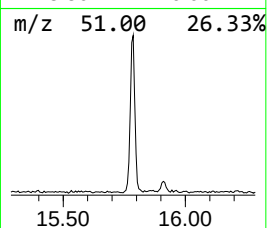
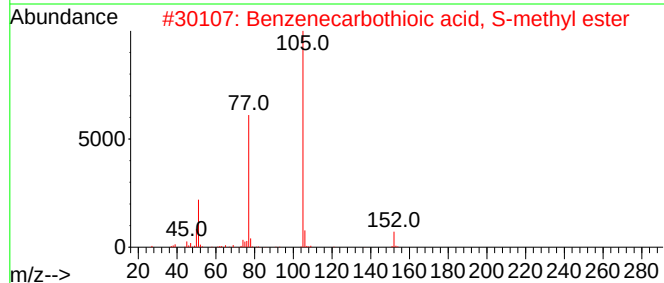
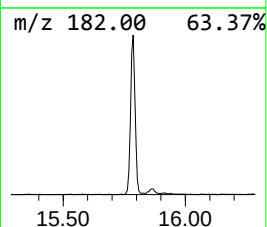
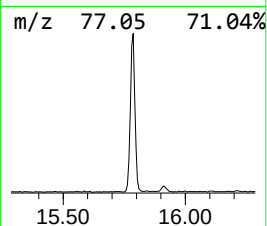
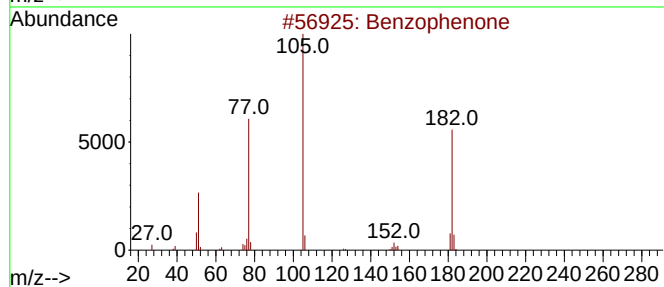
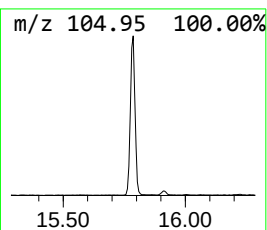
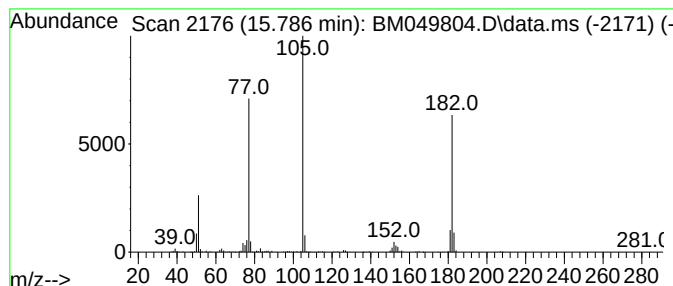
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.786	4.90 ng	620828	Acenaphthene-d10	14.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	43
4			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	43
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	43



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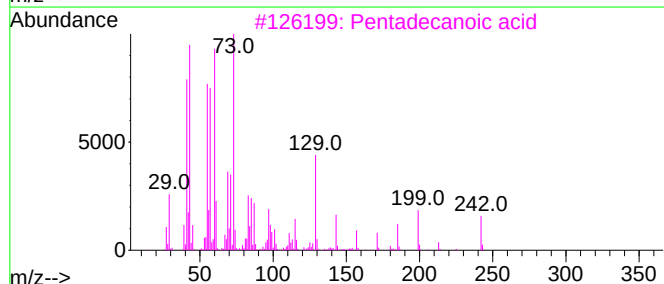
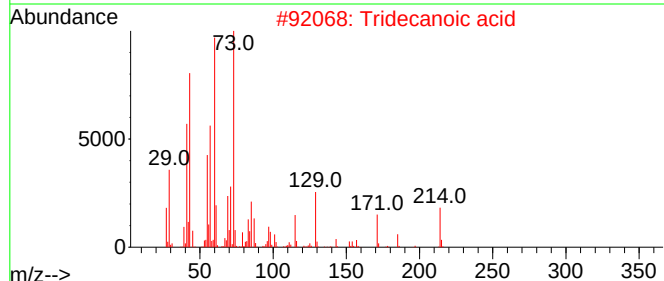
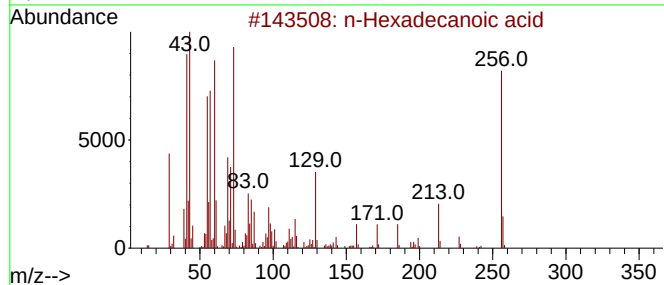
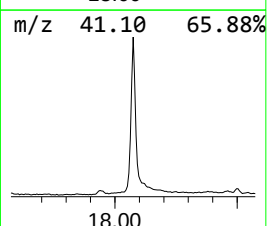
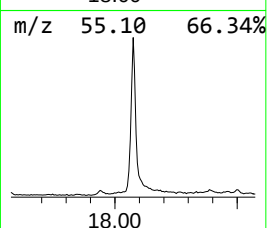
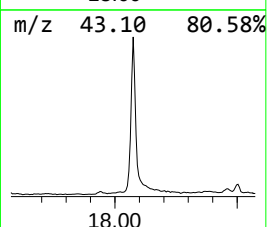
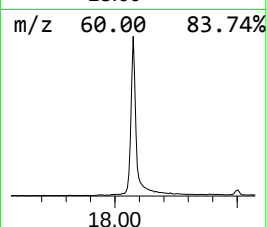
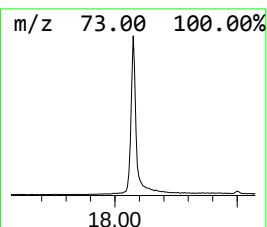
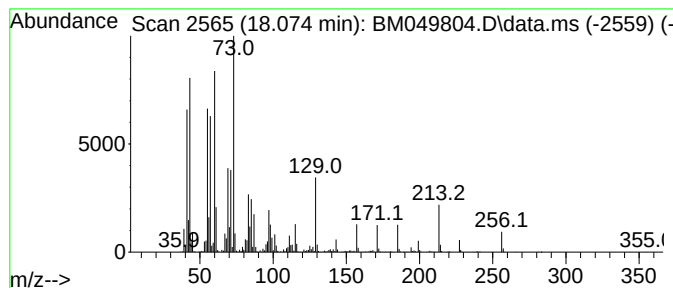
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	25.89 ng	3759070	Phenanthrene-d10	17.168

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	52



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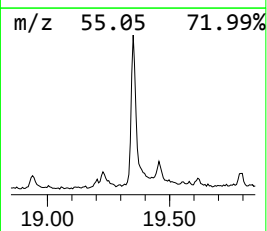
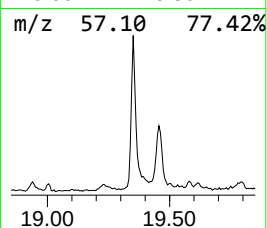
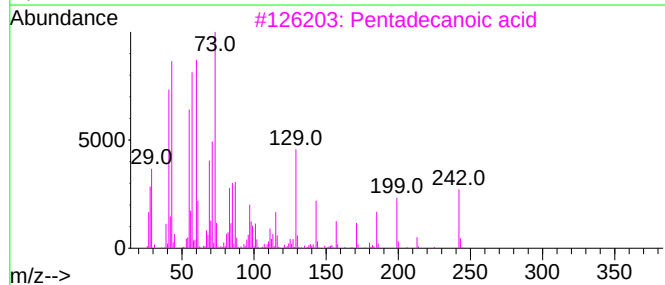
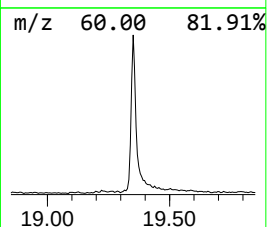
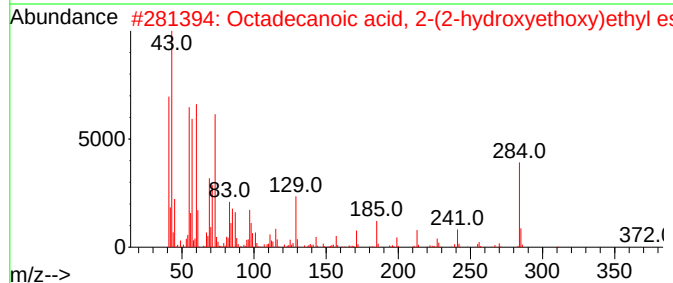
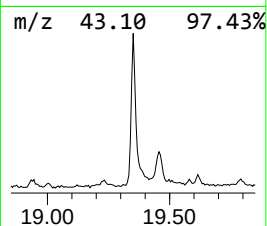
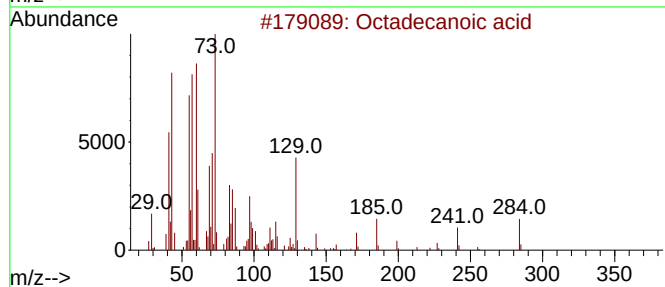
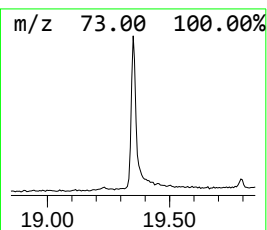
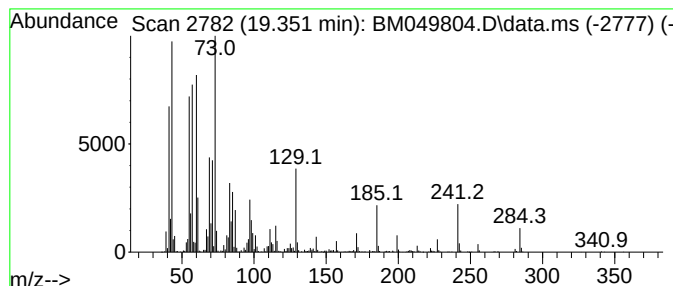
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.351	10.33 ng	1631770	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049804.D
Acq On : 03 Apr 2025 13:58
Operator : RC/JU
Sample : Q1693-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

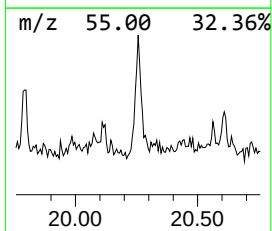
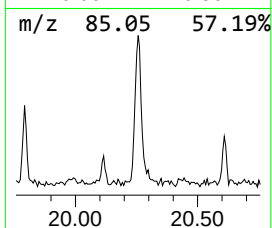
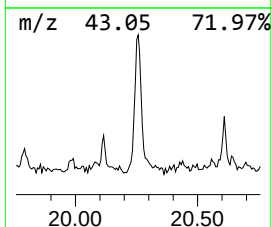
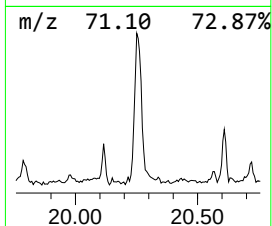
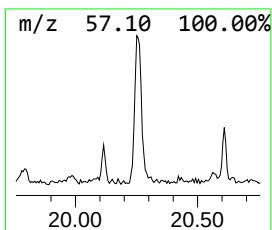
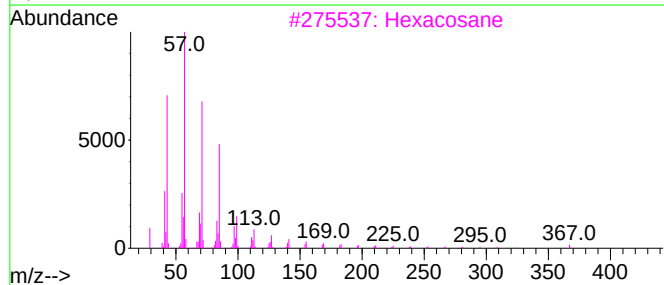
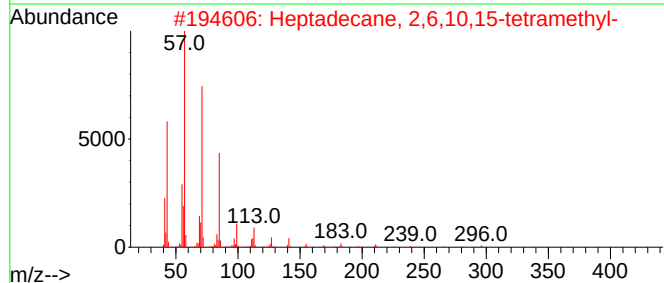
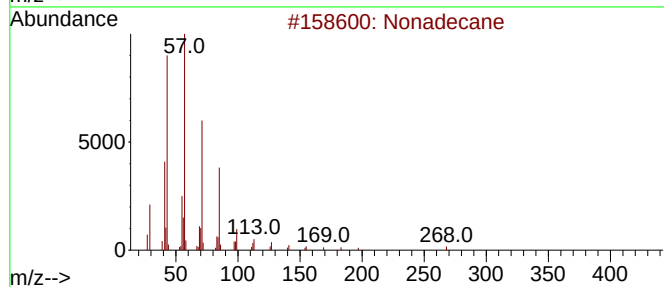
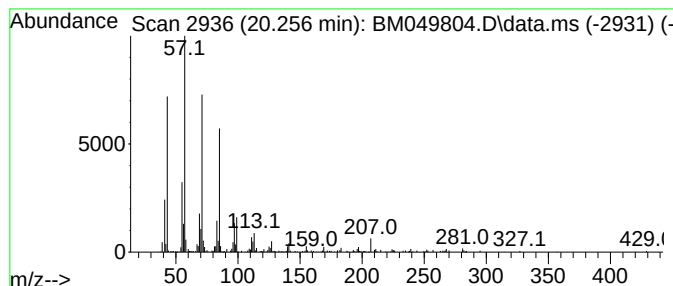
Instrument :
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ClientSampleId :
WCS-TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.256	2.16 ng	340749	Chrysene-d12	21.403	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	86
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
3	Hexacosane	366	C26H54	000630-01-3	76
4	Octacosane	394	C28H58	000630-02-4	76
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049804.D
Acq On : 03 Apr 2025 13:58
Operator : RC/JU
Sample : Q1693-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WCS-TP-3

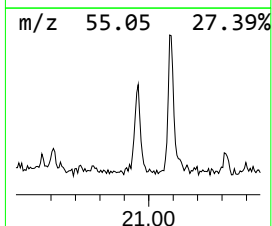
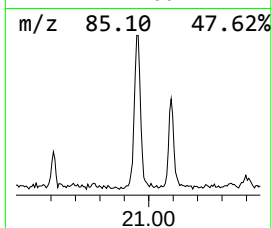
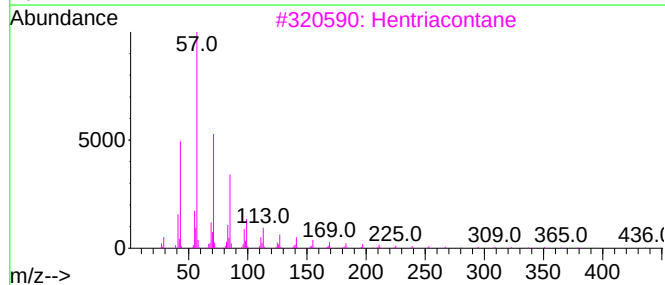
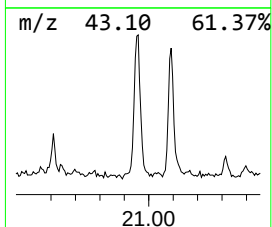
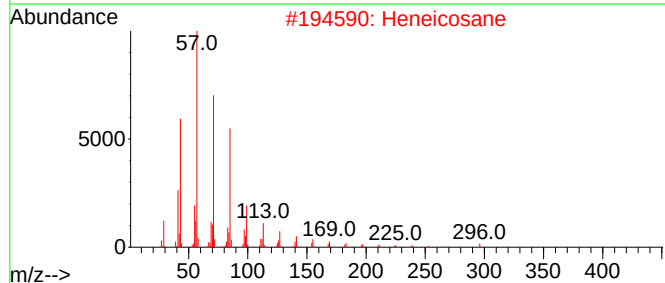
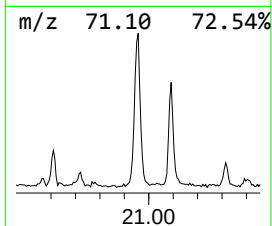
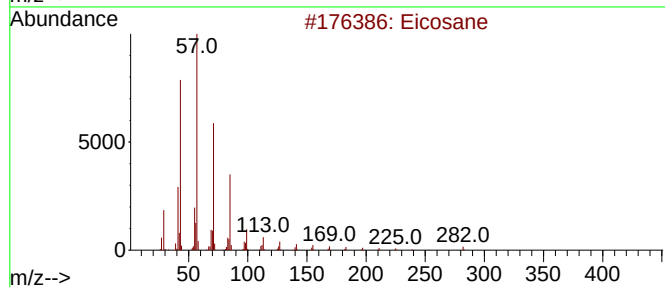
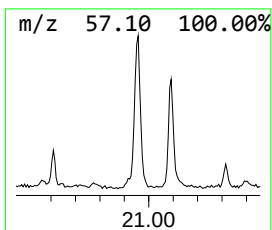
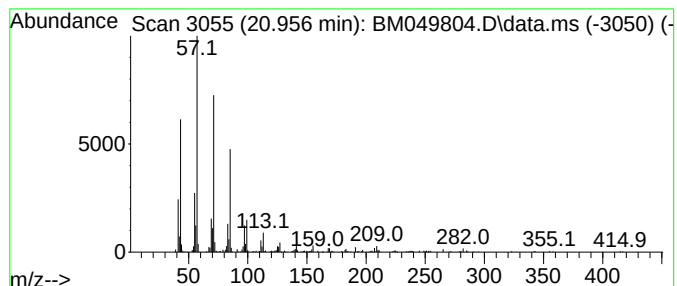
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.956	2.83 ng	446855	Chrysene-d12	21.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Heneicosane	296	C21H44	000629-94-7	87
3			Hentriacontane	437	C31H64	000630-04-6	86
4			Hexadecane	226	C16H34	000544-76-3	83
5			Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049804.D
Acq On : 03 Apr 2025 13:58
Operator : RC/JU
Sample : Q1693-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

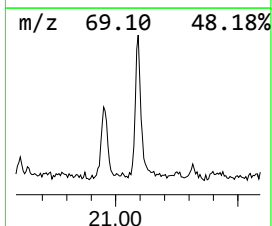
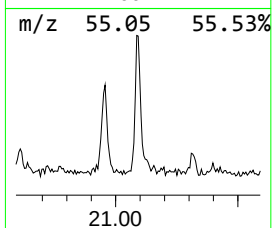
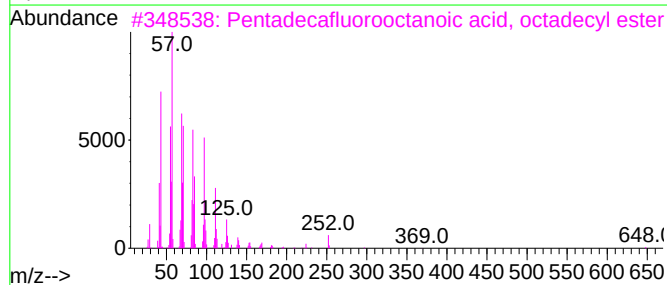
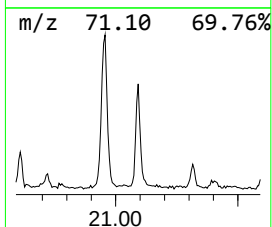
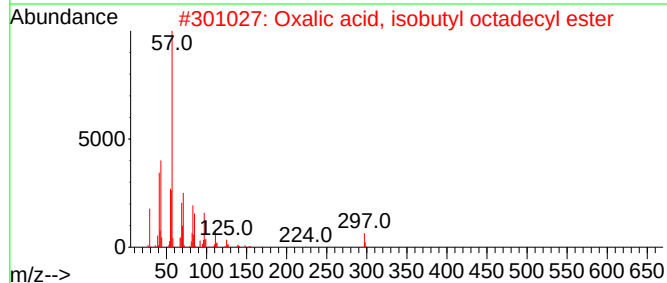
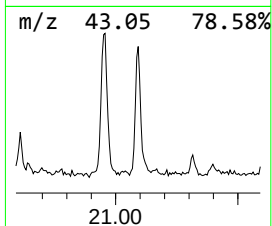
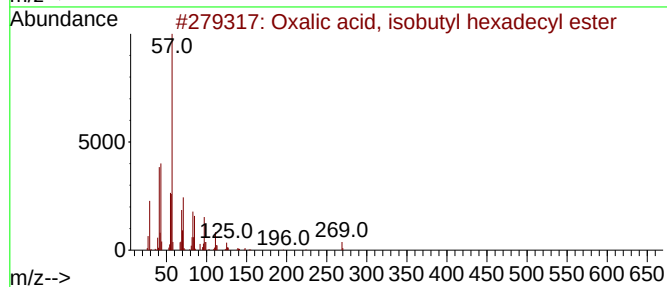
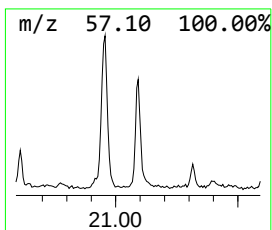
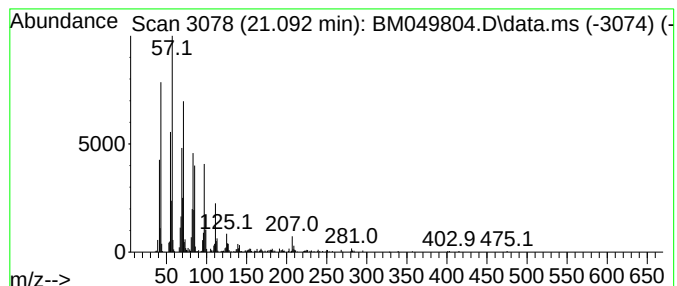
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxalic acid, isobutyl hexad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.092	2.94 ng	463857	Chrysene-d12	21.403	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
5	Eicosyl octyl ether	410	C28H58O	1000406-38-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049804.D
Acq On : 03 Apr 2025 13:58
Operator : RC/JU
Sample : Q1693-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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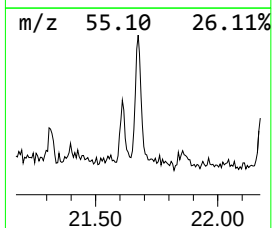
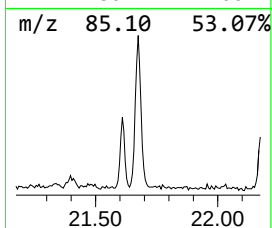
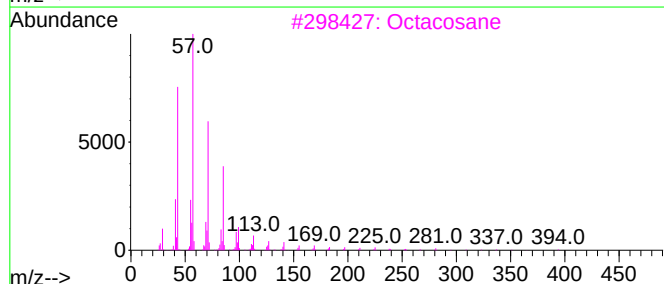
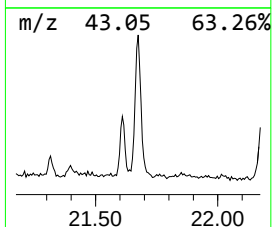
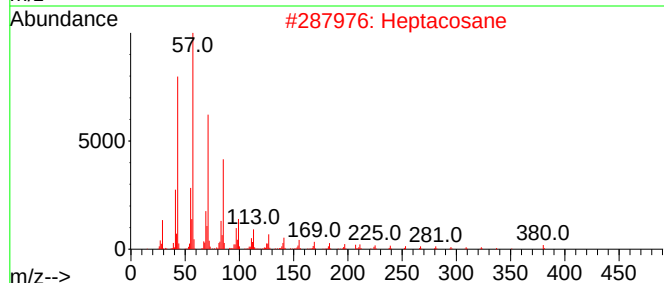
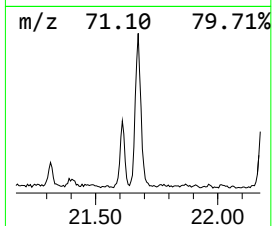
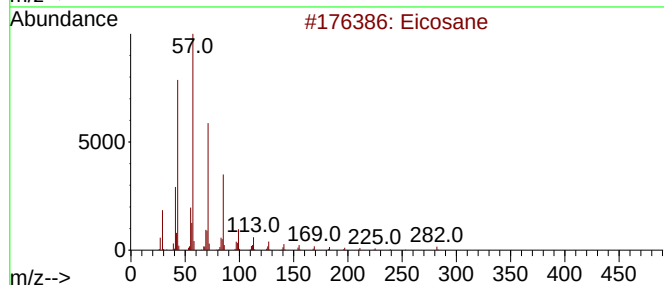
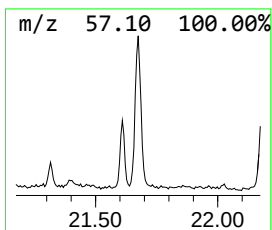
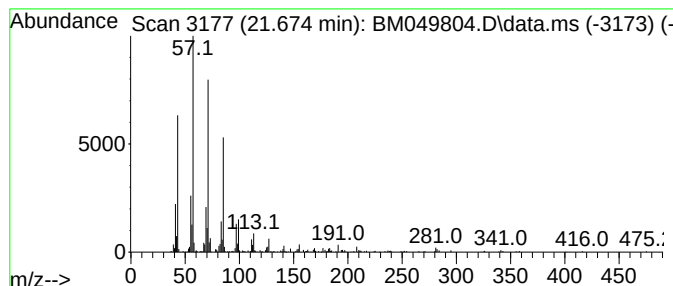
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.674	2.96 ng	468429	Chrysene-d12	21.403

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	91
2		Heptacosane	380	C27H56	000593-49-7	90
3		Octacosane	394	C28H58	000630-02-4	87
4		Hexacosane	366	C26H54	000630-01-3	86
5		Dodecane, 4-methyl-	184	C13H28	006117-97-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049804.D
Acq On : 03 Apr 2025 13:58
Operator : RC/JU
Sample : Q1693-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

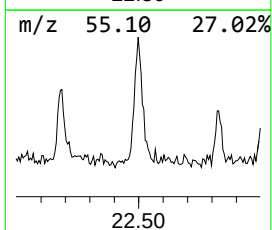
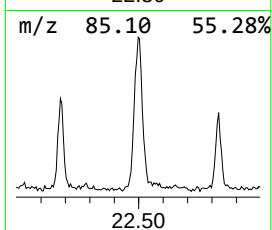
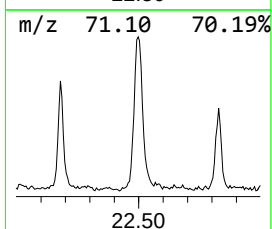
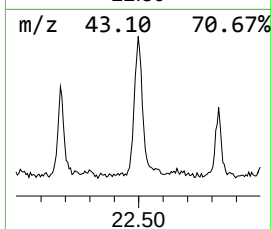
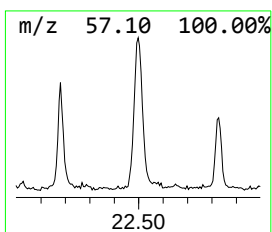
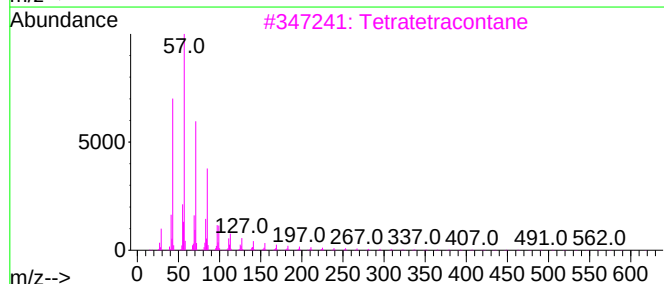
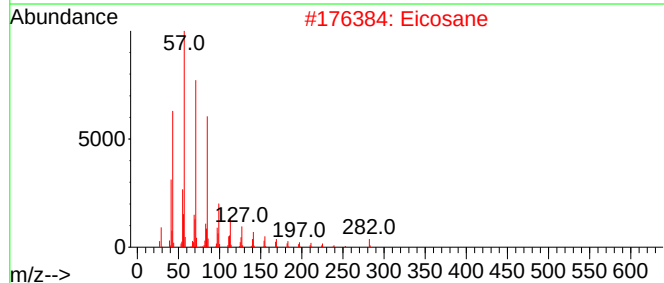
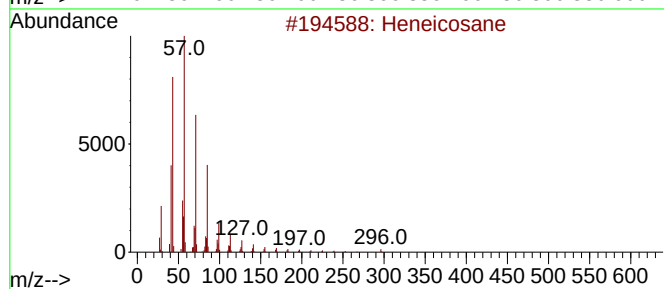
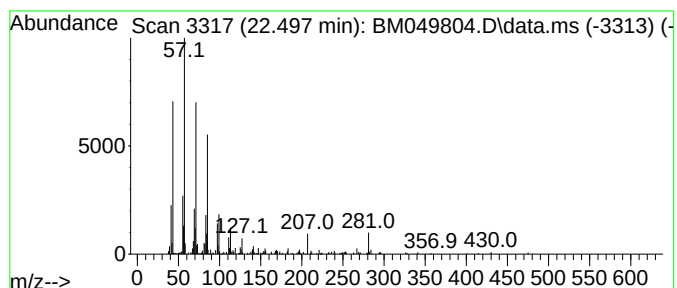
Instrument :
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ClientSampleId :
WCS-TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.497	2.84 ng	448954	Chrysene-d12	21.403	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	94
2	Eicosane	282	C20H42	000112-95-8	87
3	Tetratetracontane	619	C44H90	007098-22-8	83
4	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	80
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040325\
Data File : BM049804.D
Acq On : 03 Apr 2025 13:58
Operator : RC/JU
Sample : Q1693-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WCS-TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031325.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
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2-Pentanone, 4-...	4.905	15.0	ng	1158820	1	7.787	1548210	20.0
2-Pentanone, 4-...	5.981	2.5	ng	196800	1	7.787	1548210	20.0
Benzophenone	15.786	4.9	ng	620828	3	14.427	2531910	20.0
n-Hexadecanoic ...	18.074	25.9	ng	3759070	4	17.168	2904260	20.0
Octadecanoic acid	19.351	10.3	ng	1631770	5	21.403	3160160	20.0
Nonadecane	20.256	2.2	ng	340749	5	21.403	3160160	20.0
Eicosane	20.956	2.8	ng	446855	5	21.403	3160160	20.0
Oxalic acid, is...	21.092	2.9	ng	463857	5	21.403	3160160	20.0
Heptacosane	21.674	3.0	ng	468429	5	21.403	3160160	20.0
Heneicosane	22.497	2.8	ng	448954	5	21.403	3160160	20.0