

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
 Data File : BM049878.D
 Acq On : 10 Apr 2025 10:54
 Operator : RC/JU
 Sample : Q1753-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-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-BM040825.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM049878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	319	324	335	rVB	837205	1118165	8.68%	1.667%
2	5.363	397	404	420	rBV	3491985	5092444	39.51%	7.593%
3	5.969	502	507	515	rVB	133891	190896	1.48%	0.285%
4	6.951	666	674	685	rBV	3441776	5223777	40.53%	7.789%
5	7.775	808	814	822	rBV	993929	1534950	11.91%	2.289%
6	8.934	1003	1011	1023	rBV	1952503	3195939	24.80%	4.765%
7	10.569	1280	1289	1301	rBV	1153107	1949305	15.13%	2.907%
8	13.039	1702	1709	1720	rBV	5719880	7956260	61.74%	11.863%
9	14.421	1936	1944	1950	rBV	1827280	2676527	20.77%	3.991%
10	15.774	2168	2174	2182	rBV	1083191	1435436	11.14%	2.140%
11	15.910	2190	2197	2210	rBV	4820819	6793338	52.71%	10.129%
12	17.162	2401	2410	2419	rBV	2355586	3244353	25.17%	4.838%
13	18.062	2557	2563	2584	rBV	2472501	3833766	29.75%	5.716%
14	19.339	2776	2780	2797	rBV	1119666	1841826	14.29%	2.746%
15	19.786	2851	2856	2862	rBV	11206909	12887461	100.00%	19.216%
16	21.080	3072	3076	3086	rBV3	294235	525247	4.08%	0.783%
17	21.397	3124	3130	3136	rBV	2411616	3546067	27.52%	5.287%
18	24.391	3632	3639	3654	rVB	1537400	4020762	31.20%	5.995%

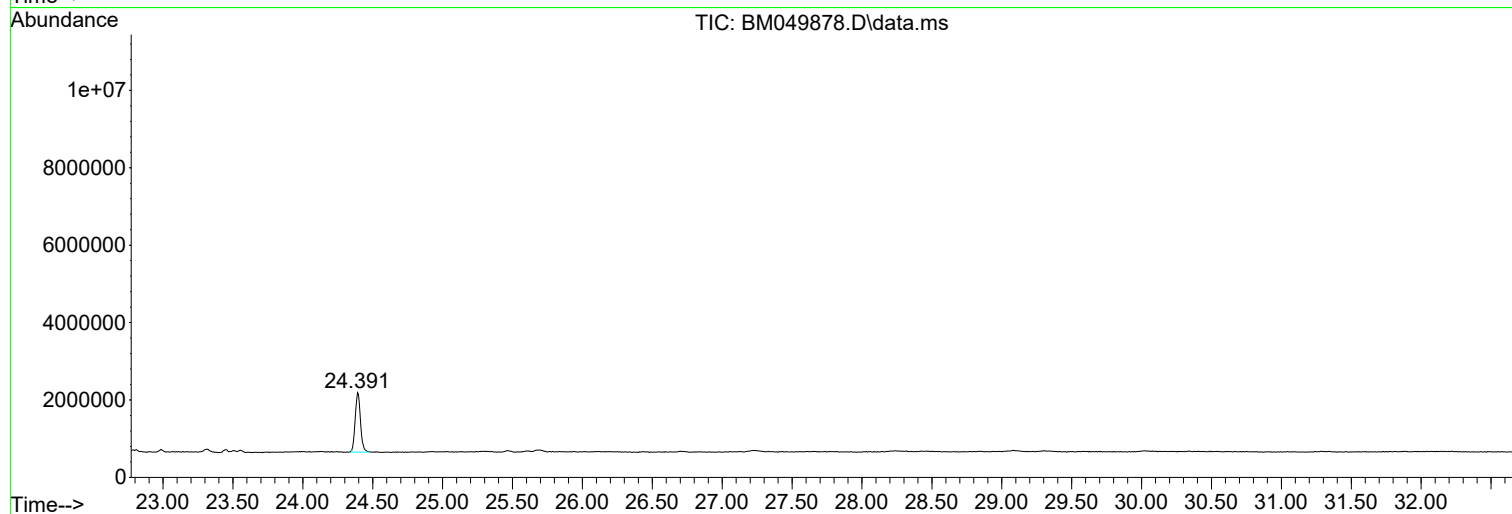
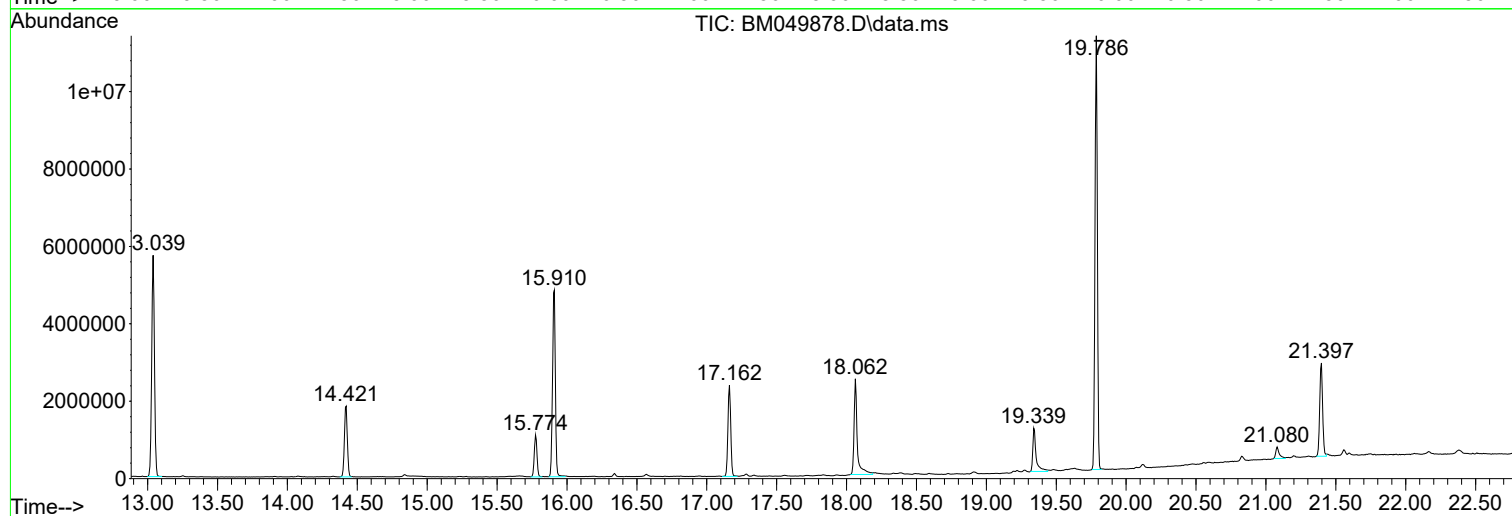
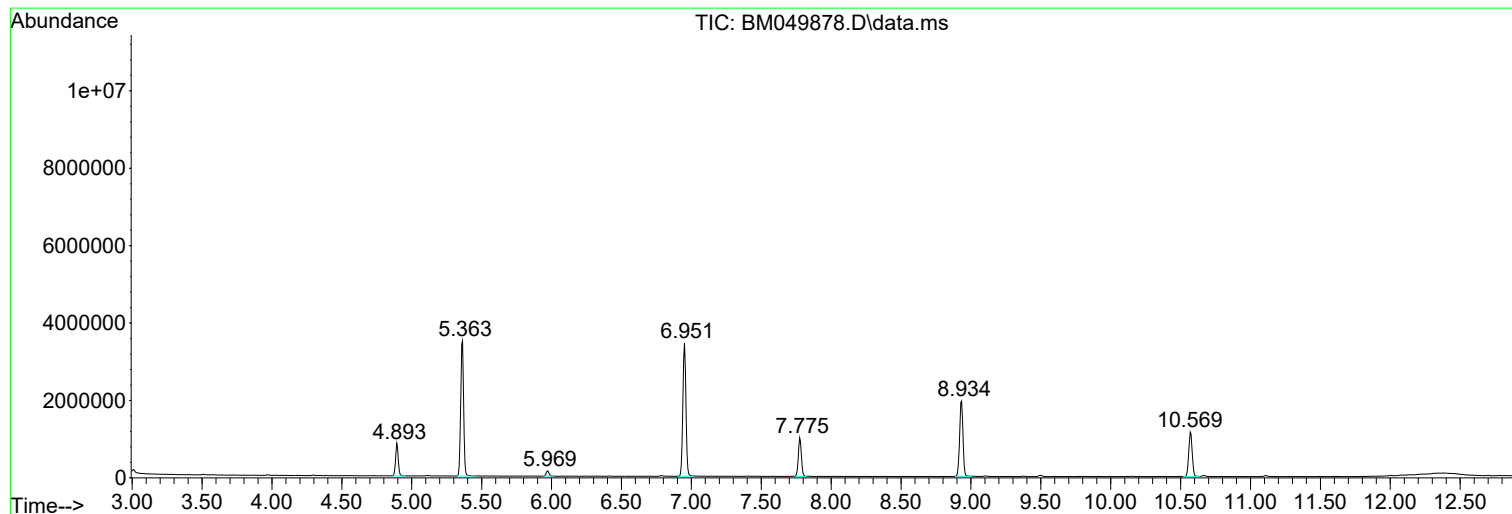
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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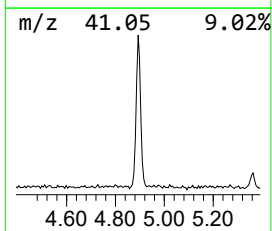
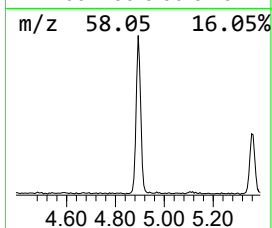
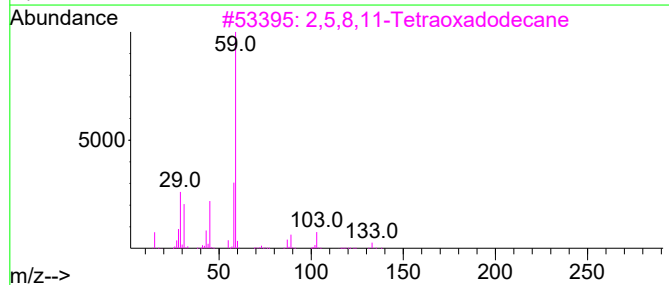
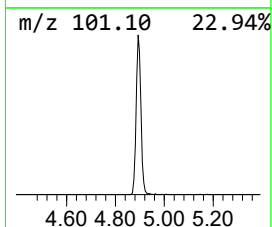
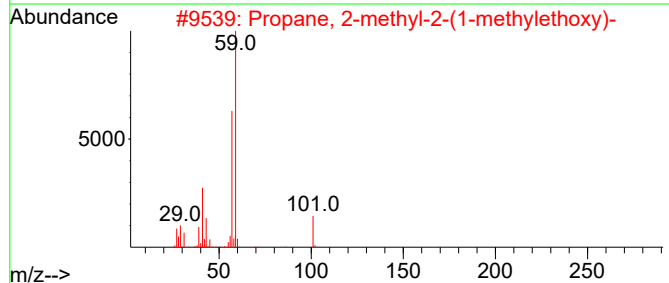
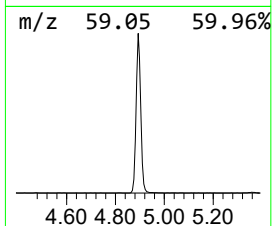
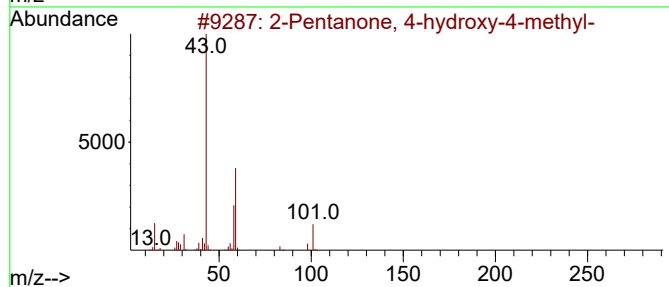
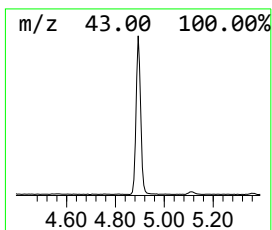
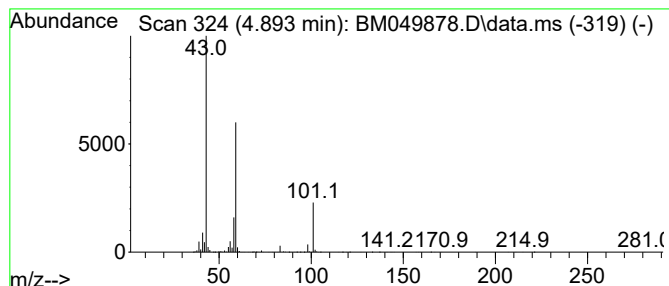
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.893	14.57 ng	1118170	1,4-Dichlorobenzene-d4	7.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50		
3	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		



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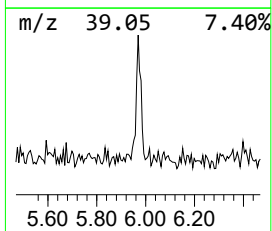
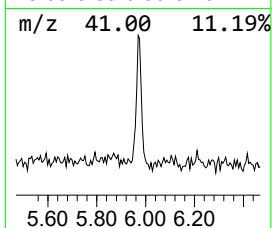
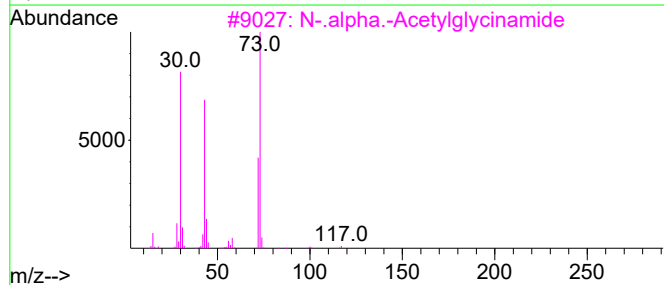
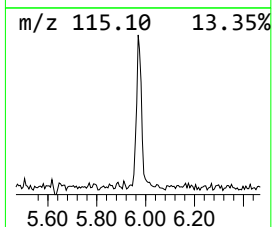
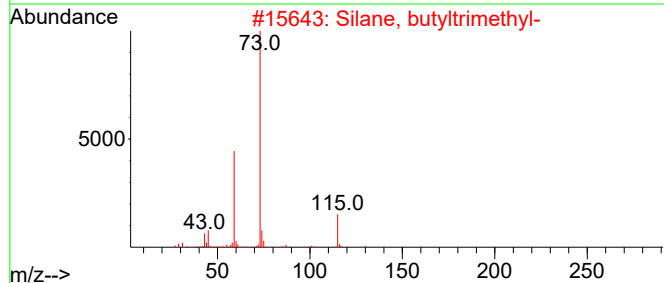
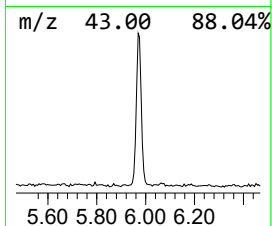
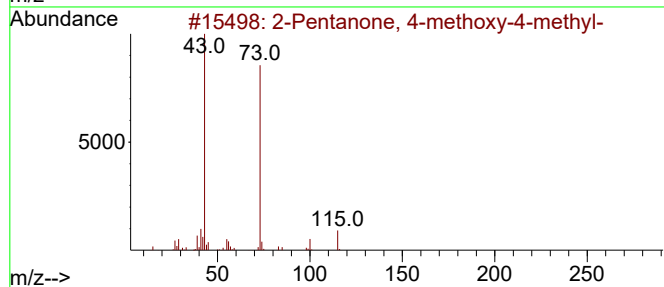
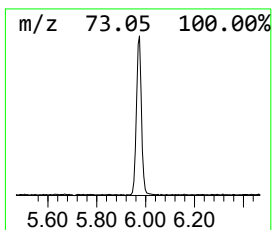
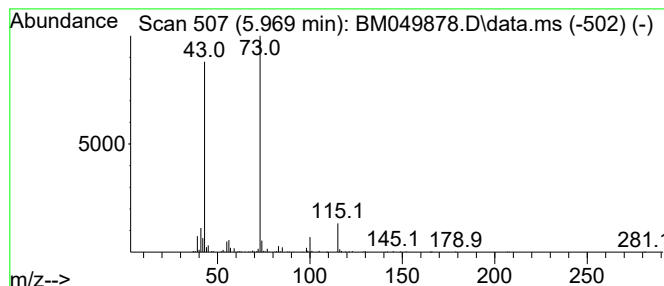
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	2.49 ng	190896	1,4-Dichlorobenzene-d4	7.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		Silane, butyltrimethyl-	130	C7H18Si	001000-49-3	37
3		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	28
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	28
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25



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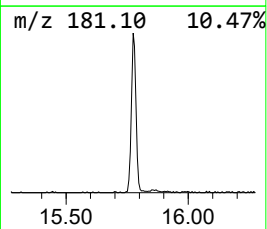
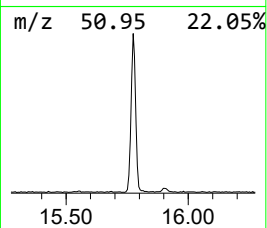
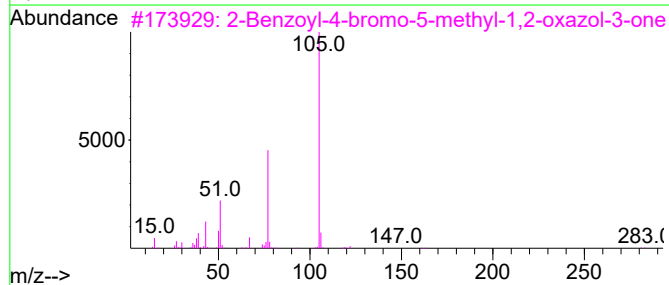
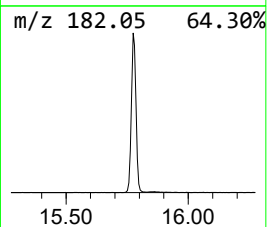
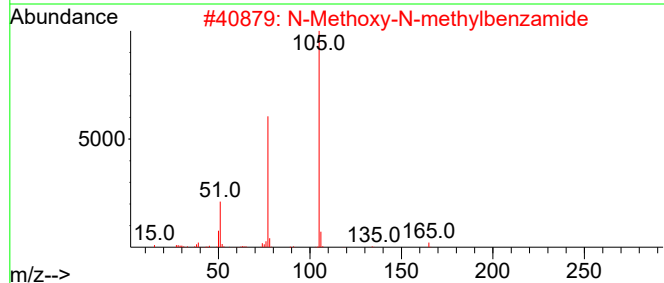
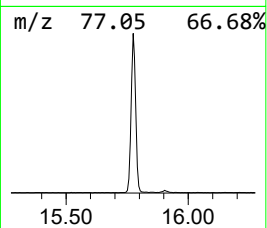
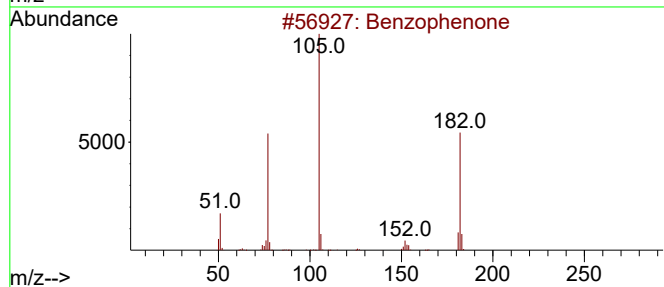
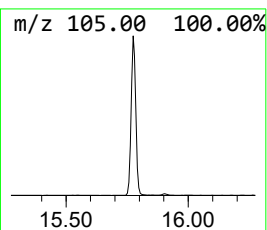
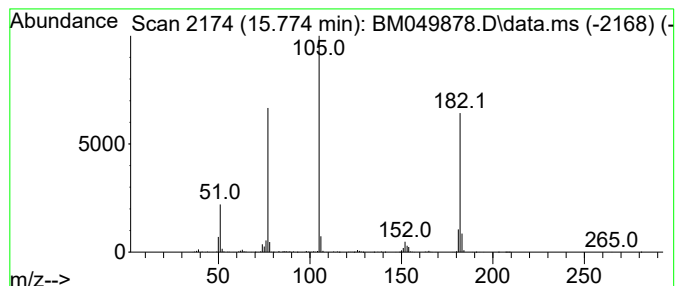
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.774	10.73 ng	1435440	Acenaphthene-d10	14.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
3			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			Benzenebutanoic acid, .gamma.-ox...	192	C11H12O3	025333-24-8	47



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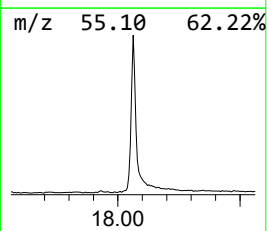
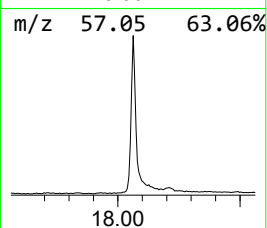
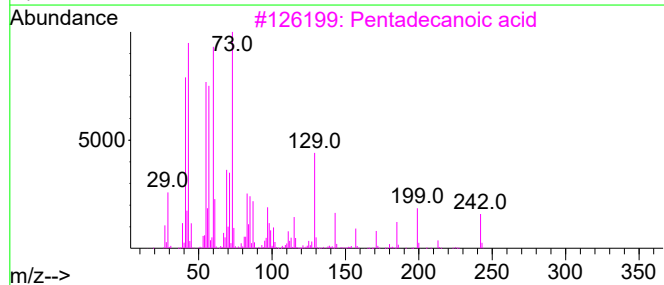
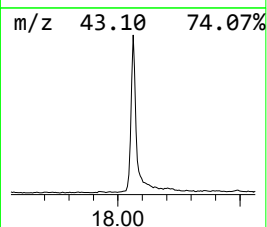
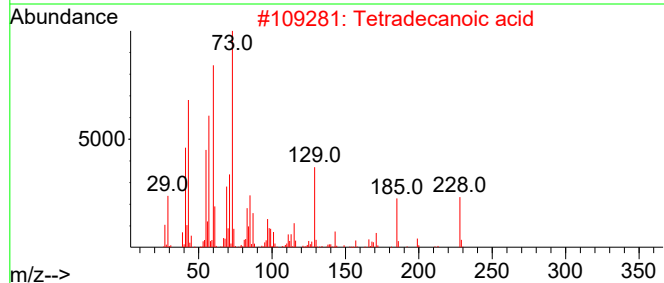
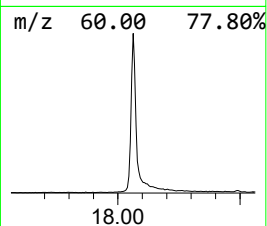
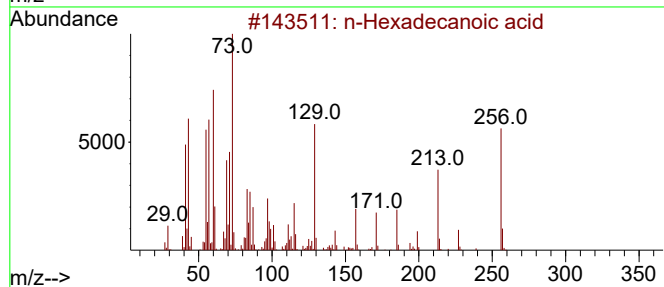
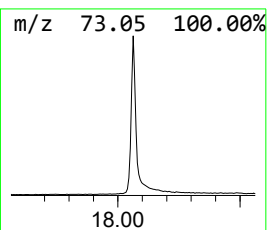
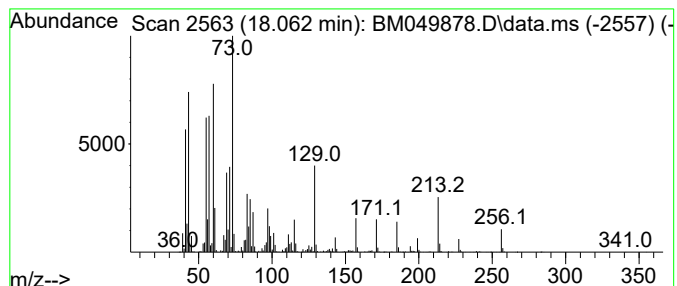
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.062	23.63 ng	3833770	Phenanthrene-d10	17.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	89
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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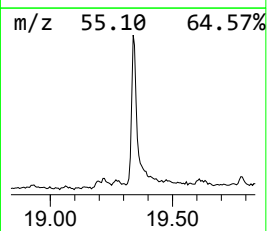
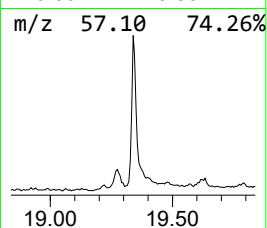
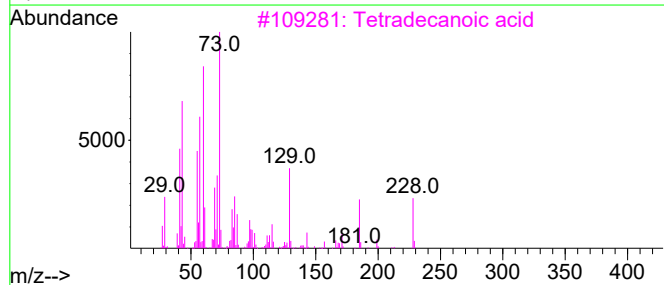
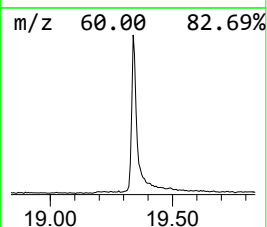
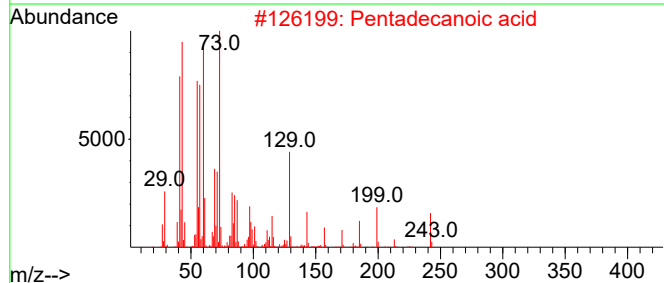
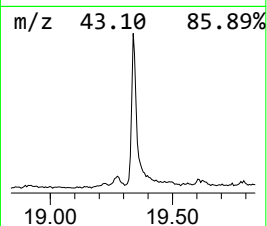
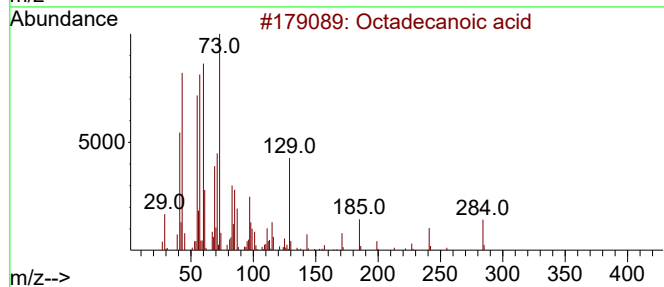
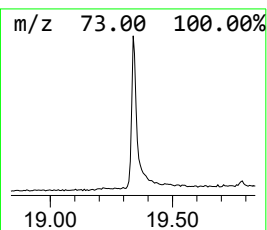
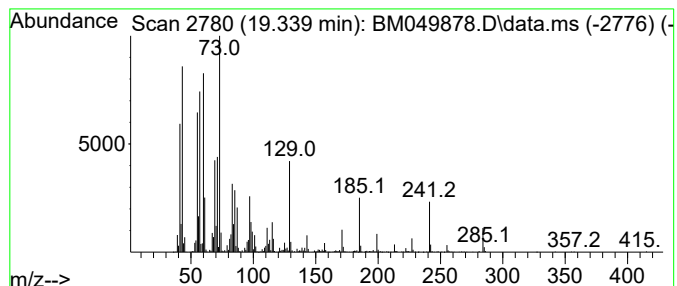
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	10.39 ng	1841830	Chrysene-d12	21.398

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



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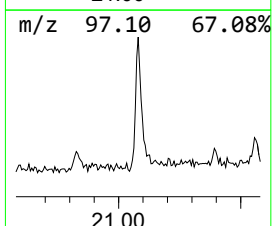
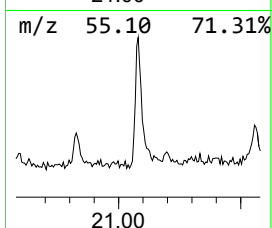
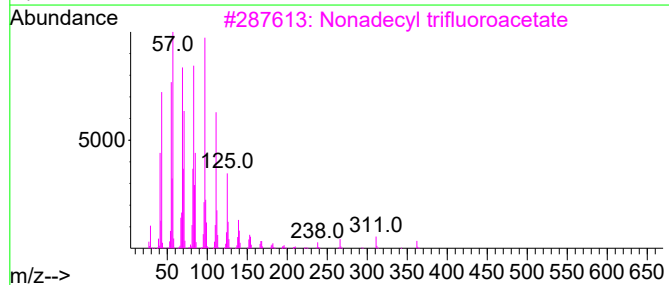
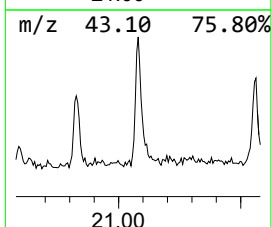
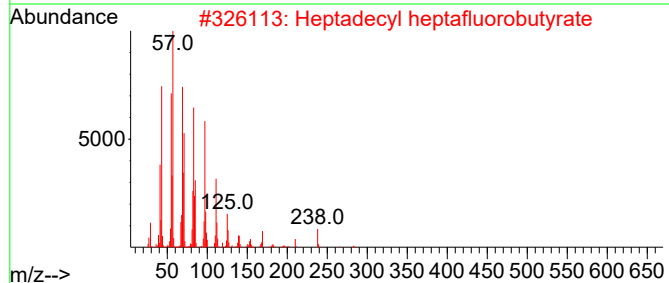
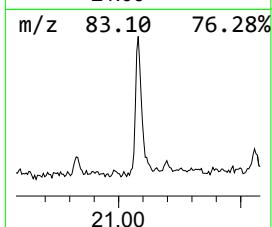
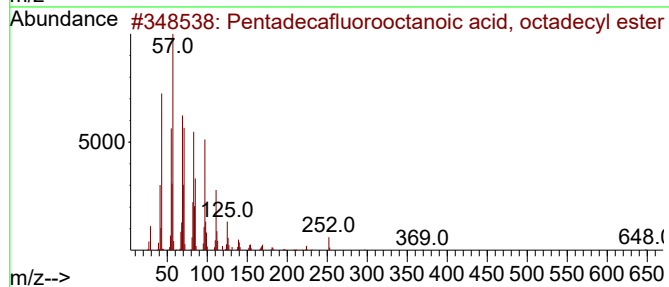
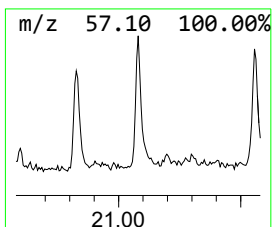
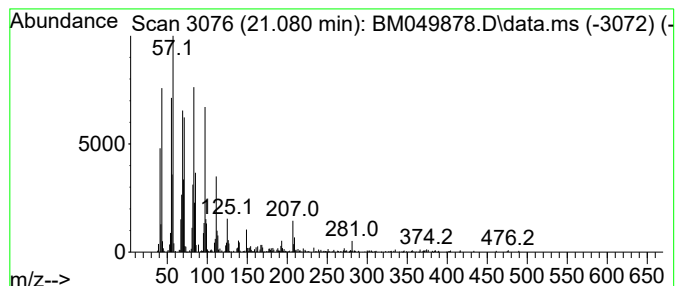
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	2.96 ng	525247	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041025\
Data File : BM049878.D
Acq On : 10 Apr 2025 10:54
Operator : RC/JU
Sample : Q1753-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040825.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
2-Pentanone, 4-...	4.893	14.6	ng	1118170	1	7.775	1534950	20.0
2-Pentanone, 4-...	5.969	2.5	ng	190896	1	7.775	1534950	20.0
Benzophenone	15.774	10.7	ng	1435440	3	14.422	2676530	20.0
n-Hexadecanoic ...	18.062	23.6	ng	3833770	4	17.163	3244350	20.0
Octadecanoic acid	19.339	10.4	ng	1841830	5	21.398	3546070	20.0
Pentadecafluoro...	21.080	3.0	ng	525247	5	21.398	3546070	20.0