

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
 Data File : BG056342.D
 Acq On : 19 Jan 2023 00:16
 Operator : CG/JU
 Sample : 01184-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 APNB-EAST

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_G\Methods\8270-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056342.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.317	3	5	18	rVB	140922	171081	6.76%	1.425%
2	5.344	343	350	359	rBB	125380	189807	7.50%	1.581%
3	5.826	424	432	442	rBV	519425	827009	32.69%	6.890%
4	7.448	700	708	719	rBV	519418	901646	35.64%	7.512%
5	8.306	846	854	862	rBB	131698	223977	8.85%	1.866%
6	9.481	1046	1054	1064	rBB	313866	553466	21.88%	4.611%
7	11.138	1327	1336	1344	rBV	172425	321256	12.70%	2.677%
8	13.546	1738	1746	1753	rBV	1162999	1763955	69.72%	14.696%
9	14.915	1973	1979	1986	rBV	342369	524462	20.73%	4.370%
10	16.255	2202	2207	2213	rVB2	23998	35125	1.39%	0.293%
11	16.396	2225	2231	2241	rBV	834607	1259241	49.77%	10.491%
12	17.653	2438	2445	2450	rBV	450934	668478	26.42%	5.569%
13	17.695	2450	2452	2459	rVB	19736	27316	1.08%	0.228%
14	18.499	2584	2589	2597	rBV2	123477	179246	7.08%	1.493%
15	19.686	2787	2791	2796	rVB	59883	85910	3.40%	0.716%
16	19.757	2799	2803	2810	rVV4	36961	57873	2.29%	0.482%
17	20.045	2849	2852	2858	rVB	52710	74873	2.96%	0.624%
18	20.233	2878	2884	2889	rBV	1893125	2530080	100.00%	21.080%
19	21.525	3100	3104	3113	rVB3	113965	184021	7.27%	1.533%
20	21.948	3169	3176	3182	rBV	399952	710706	28.09%	5.921%
21	25.380	3751	3760	3771	rBV2	240481	713033	28.18%	5.941%

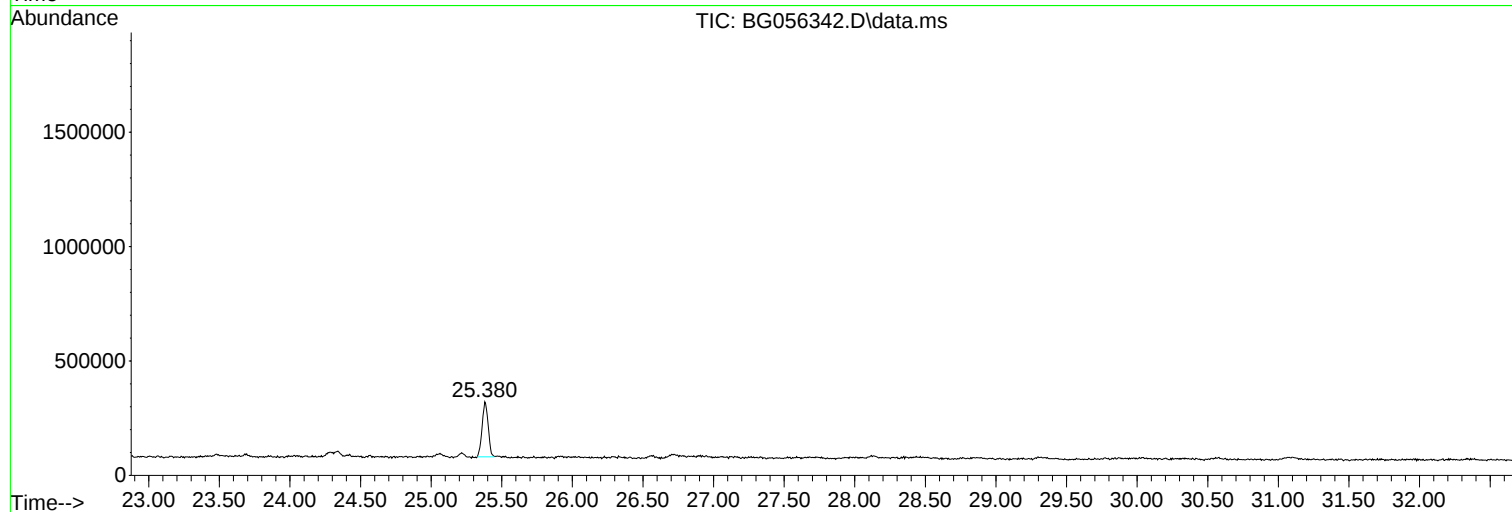
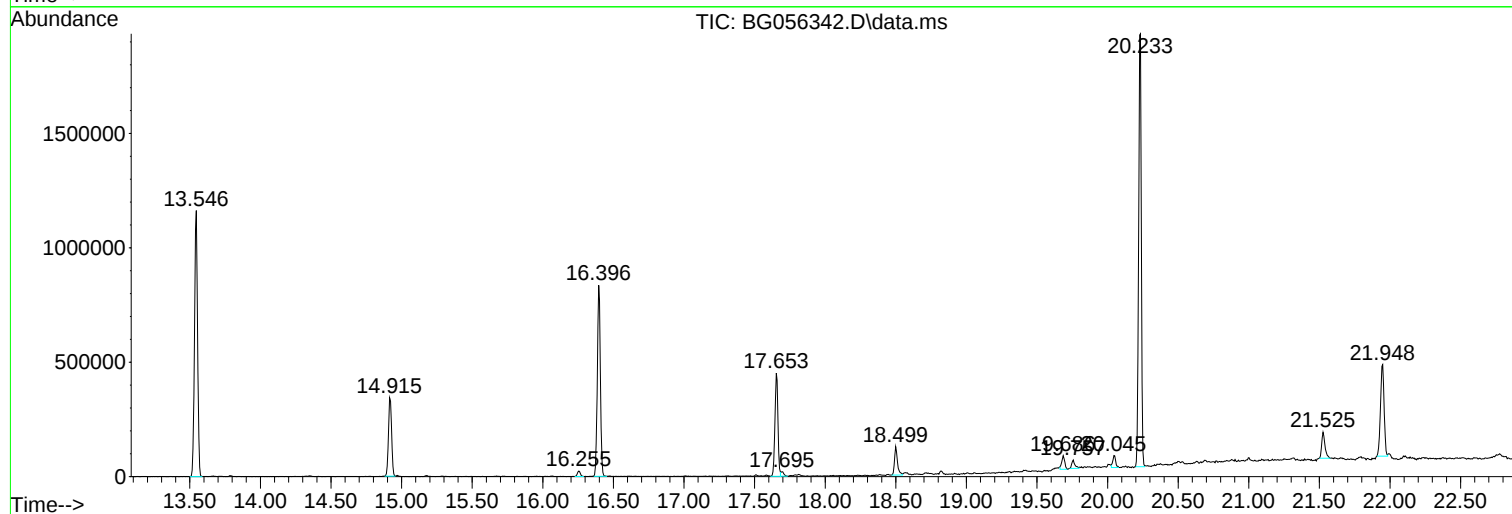
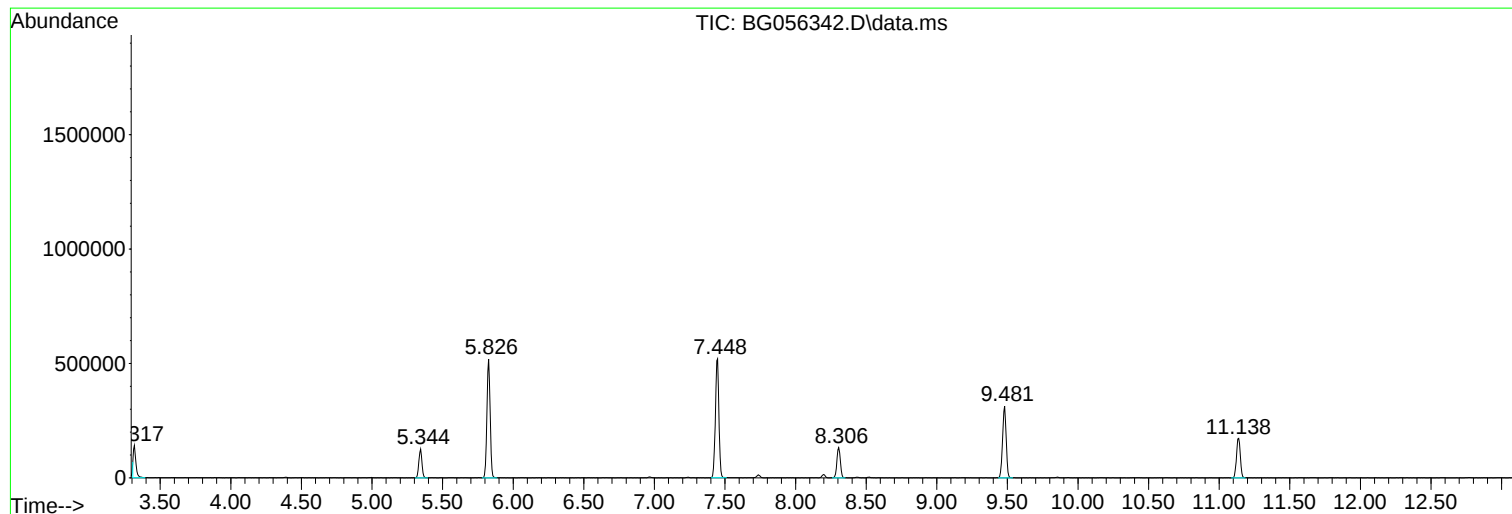
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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Instrument :
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ClientSampleId :
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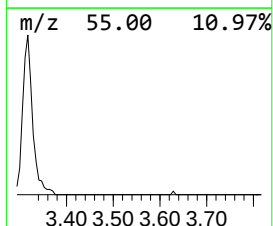
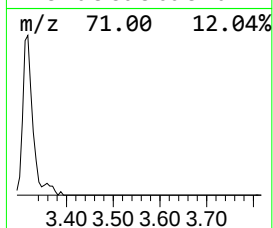
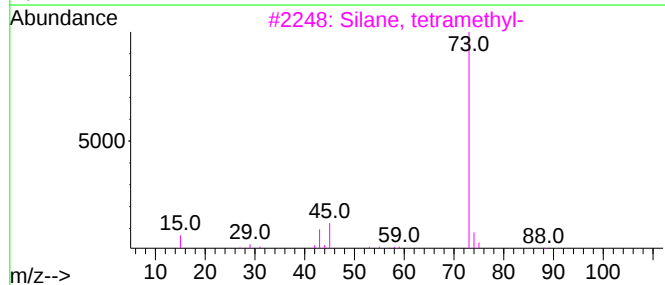
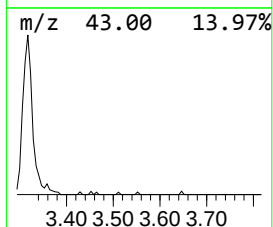
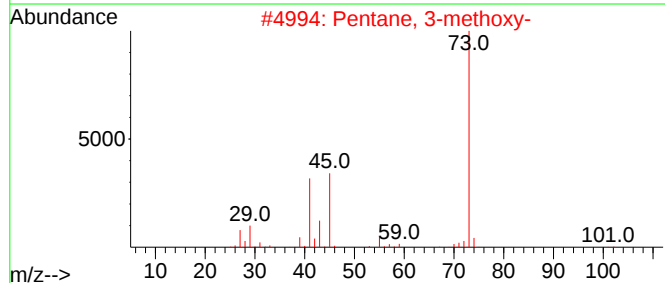
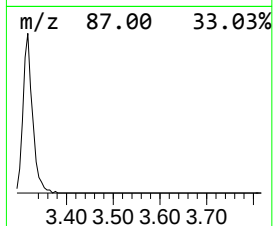
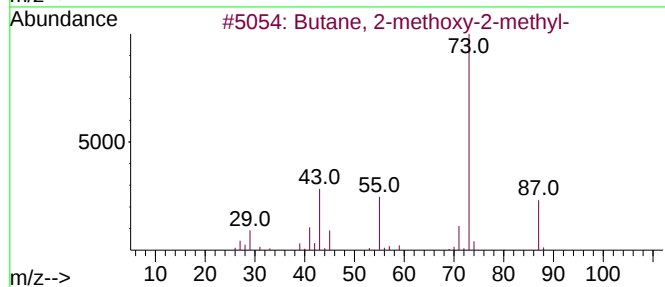
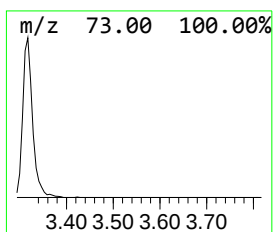
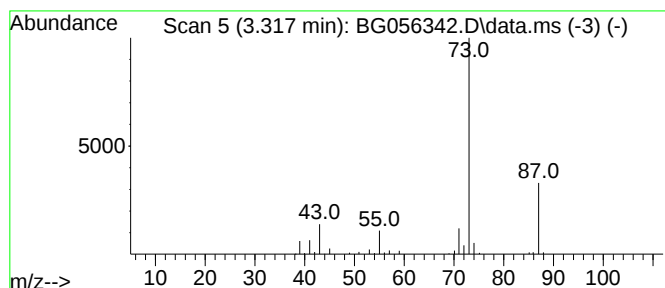
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.317	15.28 ng	171081	1,4-Dichlorobenzene-d4	8.306

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7



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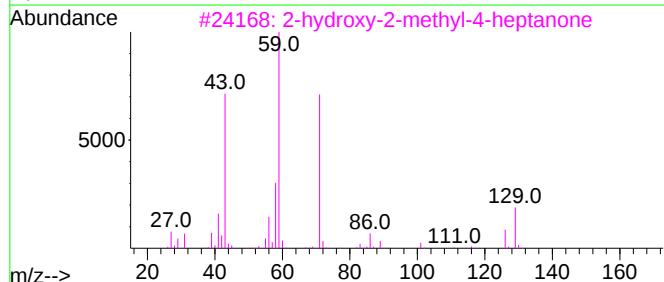
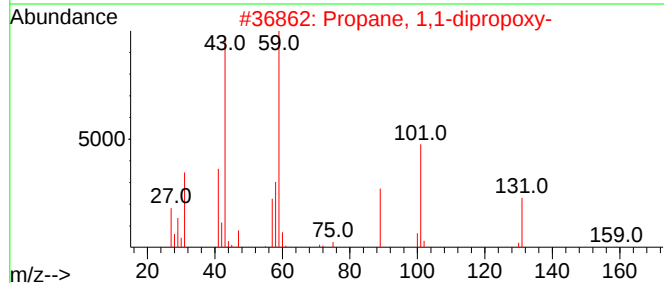
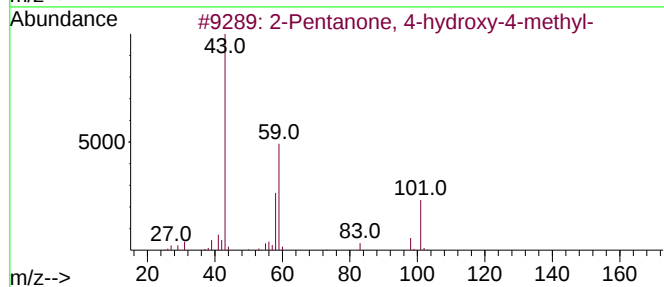
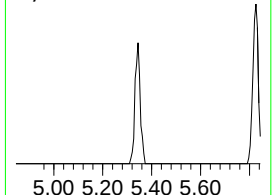
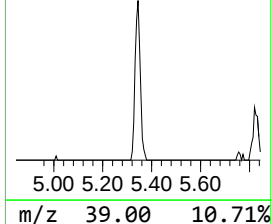
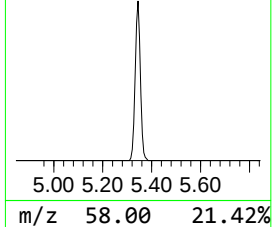
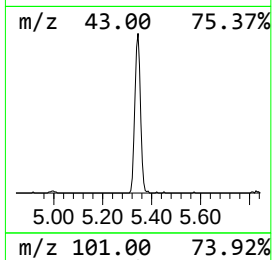
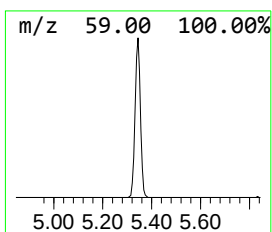
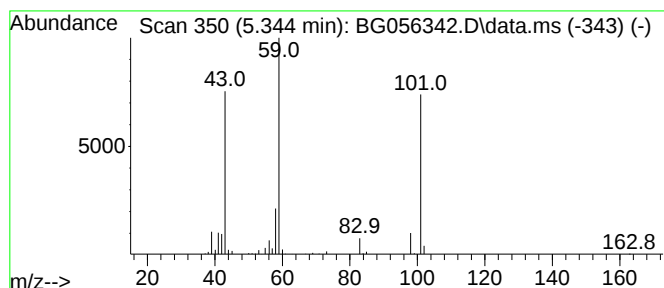
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.344	16.95 ng	189807	1,4-Dichlorobenzene-d4	8.306	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	39
3	2-hydroxy-2-methyl-4-heptanone	144	C8H16O2	054862-91-8	23
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	22
5	Tetraglyme	222	C10H22O5	000143-24-8	17



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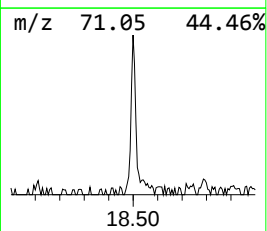
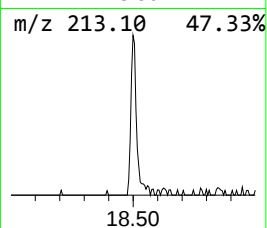
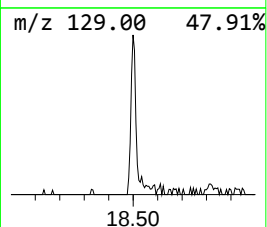
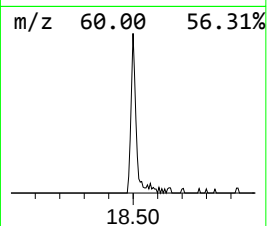
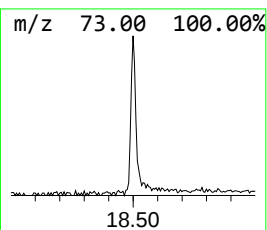
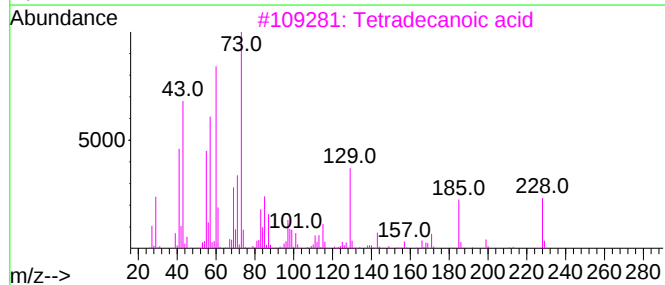
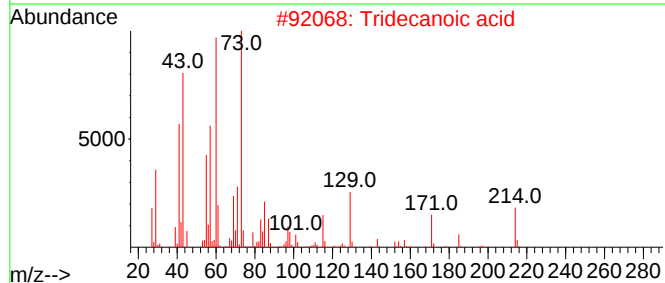
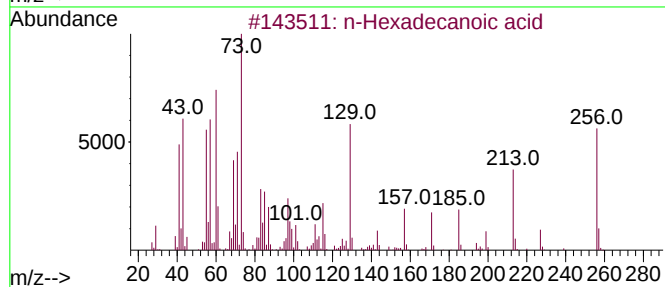
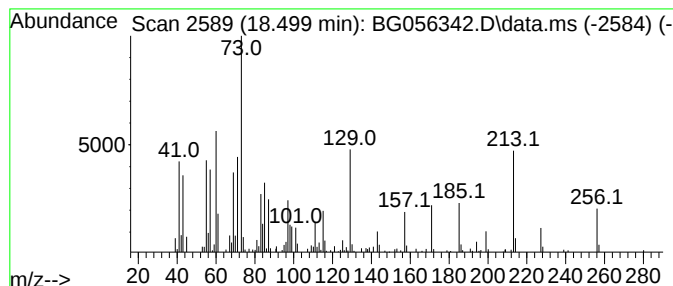
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.500	5.36 ng	179246	Phenanthrene-d10	17.653

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	55
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	38
5			Dodecanoic acid	200	C12H24O2	000143-07-7	22



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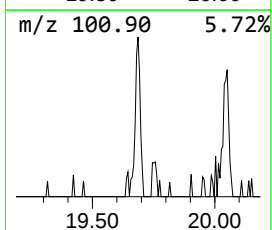
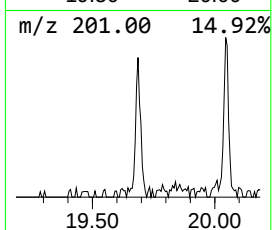
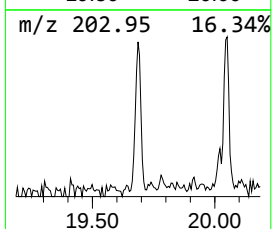
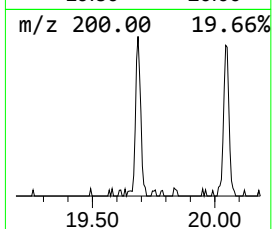
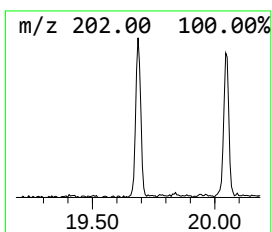
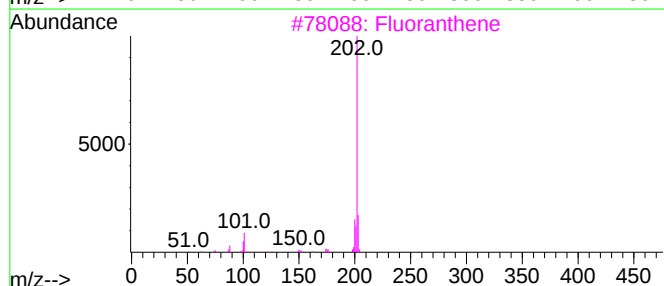
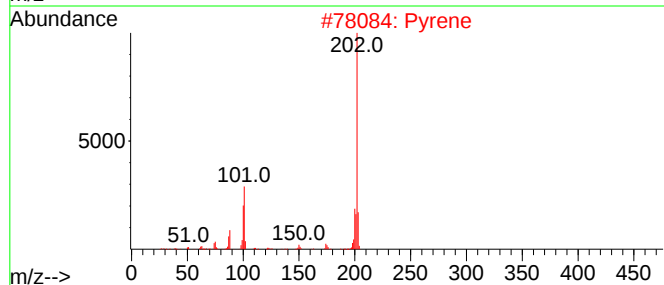
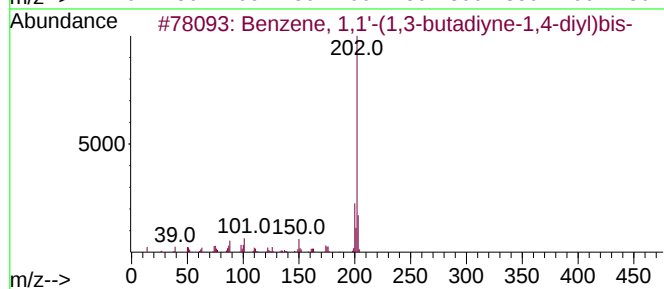
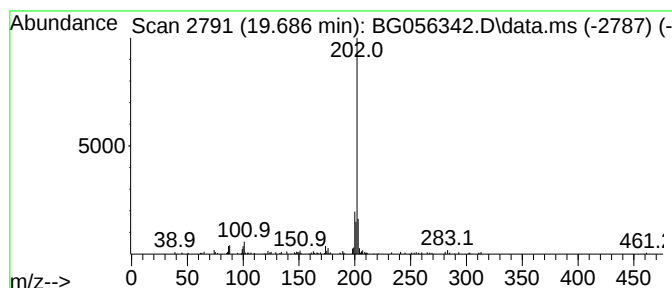
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.686	2.57 ng	85910	Phenanthrene-d10	17.653	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
2	Pyrene	202	C16H10	000129-00-0	68
3	Fluoranthene	202	C16H10	000206-44-0	64
4	5-(4-Methylphenyl)furan-2-carbox...	202	C12H10O3	1000305-27-5	53
5	4-Methoxy-naphthalene-1-carboxyl...	202	C12H10O3	1000317-85-4	40



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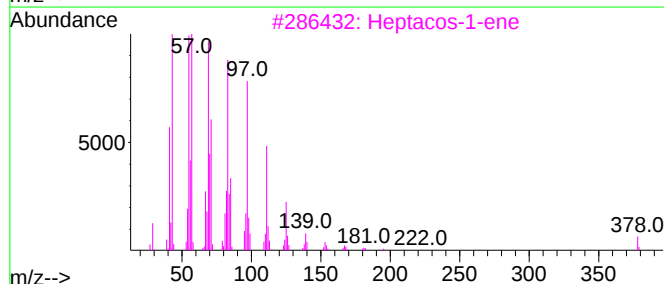
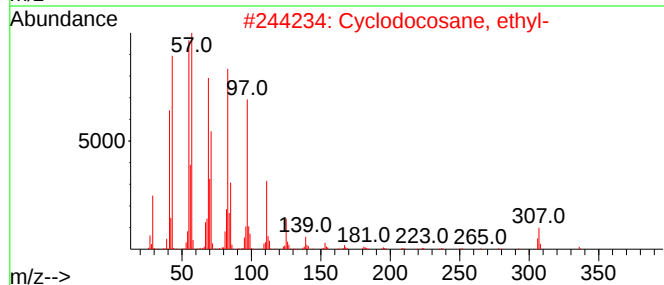
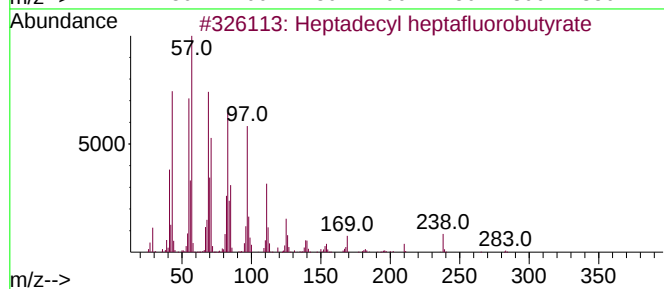
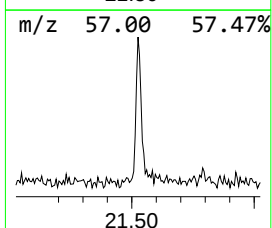
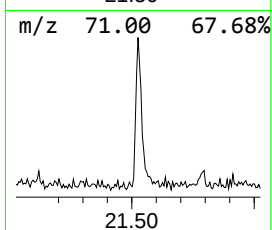
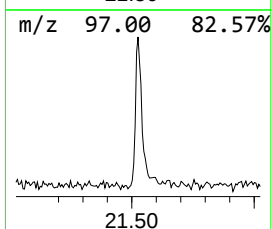
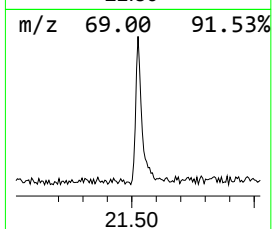
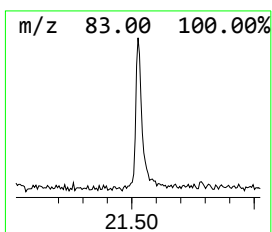
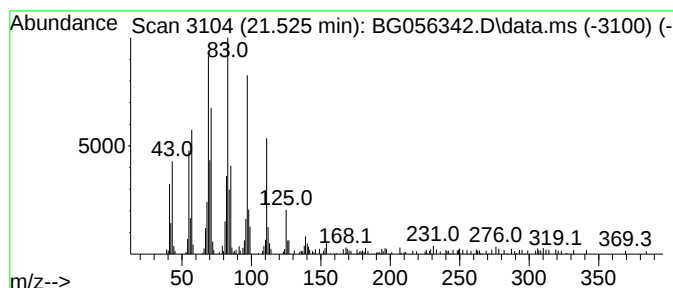
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.525	5.18 ng	184021	Chrysene-d12	21.948

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
3			Heptacos-1-ene	378	C27H54	015306-27-1	91
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.317	15.3	ng	171081	1	8.306	223977	20.0
2-Pentanone, 4-...	5.344	16.9	ng	189807	1	8.306	223977	20.0
n-Hexadecanoic ...	18.500	5.4	ng	179246	4	17.653	668478	20.0
Benzene, 1,1'-(...	19.686	2.6	ng	85910	4	17.653	668478	20.0
Heptadecyl hept...	21.525	5.2	ng	184021	5	21.948	710706	20.0