

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
 Data File : BP008737.D
 Acq On : 07 Jan 2022 21:15
 Operator : CG/JU
 Sample : N1069-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PX-2-010522

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_P\Methods\8270E-BP010622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.069	9	14	31	rVB	2094542	3230829	12.40%	1.322%
2	4.987	334	340	349	rVB2	162666	270495	1.04%	0.111%
3	5.451	412	419	434	rBV	6375205	9943866	38.17%	4.068%
4	7.045	681	690	707	rBV	6190166	10413937	39.97%	4.260%
5	7.869	823	830	838	rBV	1511965	2422485	9.30%	0.991%
6	9.028	1013	1027	1038	rBV	4088824	6964808	26.73%	2.849%
7	10.457	1262	1270	1291	rBV	351728	729248	2.80%	0.298%
8	10.669	1298	1306	1313	rBV	1975501	3459387	13.28%	1.415%
9	13.133	1717	1725	1741	rBV	10601594	16025451	61.51%	6.555%
10	14.504	1951	1958	1964	rBV	3033054	4652090	17.86%	1.903%
11	14.569	1964	1969	1977	rVB	385974	604527	2.32%	0.247%
12	15.557	2131	2137	2148	rVB	284229	458805	1.76%	0.188%
13	15.998	2205	2212	2234	rBV	8875067	13621397	52.28%	5.572%
14	17.074	2391	2395	2400	rVB	214788	334240	1.28%	0.137%
15	17.263	2418	2427	2430	rVV	3786119	6026992	23.13%	2.465%
16	17.304	2430	2434	2440	rVV	4795250	6919000	26.56%	2.830%
17	17.392	2440	2449	2455	rVB	1064574	1674449	6.43%	0.685%
18	17.663	2487	2495	2500	rBV2	580327	956252	3.67%	0.391%
19	18.045	2554	2560	2565	rBV2	504421	876731	3.36%	0.359%
20	18.098	2565	2569	2571	rVV	279227	479615	1.84%	0.196%
21	18.127	2571	2574	2576	rVV	510560	696409	2.67%	0.285%
22	18.157	2576	2579	2588	rVV2	1241572	2613570	10.03%	1.069%
23	18.251	2591	2595	2600	rVV	262213	416249	1.60%	0.170%
24	18.315	2600	2606	2610	rVV3	1029642	1711837	6.57%	0.700%
25	18.351	2610	2612	2618	rVB	334500	388955	1.49%	0.159%
26	18.610	2652	2656	2659	rBV	440288	555647	2.13%	0.227%
27	18.645	2659	2662	2667	rVB	442493	577907	2.22%	0.236%
28	19.015	2721	2725	2729	rBV2	249064	358225	1.37%	0.147%
29	19.151	2744	2748	2755	rBV	263975	422917	1.62%	0.173%
30	19.268	2762	2768	2777	rBV	11335554	16119605	61.87%	6.594%
31	19.386	2786	2788	2796	rVB2	338804	514983	1.98%	0.211%
32	19.504	2805	2808	2812	rVB	264497	322655	1.24%	0.132%
33	19.621	2818	2828	2836	rBV	9759903	16064111	61.66%	6.571%
34	19.692	2836	2840	2847	rVB2	330906	526854	2.02%	0.216%
35	19.821	2854	2862	2867	rBV	20478106	26054543	100.00%	10.658%
36	19.857	2867	2868	2875	rVB	542542	491876	1.89%	0.201%

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Min Area: 3 % of largest Peak

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	19.933	2876	2881	2888	rBV4	450407	1127898	4.33%	0.461%
38	20.074	2899	2905	2906	rVV4	344865	574956	2.21%	0.235%
39	20.104	2906	2910	2916	rVB	1283654	1790037	6.87%	0.732%
40	20.204	2922	2927	2931	rBV	1031119	1367907	5.25%	0.560%
41	20.256	2931	2936	2940	rVV2	661390	1137367	4.37%	0.465%
42	20.298	2940	2943	2946	rVV	316577	354822	1.36%	0.145%
43	20.398	2956	2960	2963	rBV	336132	418628	1.61%	0.171%
44	20.439	2963	2967	2971	rBV3	362538	509638	1.96%	0.208%
45	20.833	3031	3034	3041	rVB	583294	822425	3.16%	0.336%
46	20.998	3057	3062	3066	rBV2	780719	1309096	5.02%	0.535%
47	21.039	3066	3069	3070	rVV	848784	933408	3.58%	0.382%
48	21.062	3070	3073	3080	rVV3	1312650	2943564	11.30%	1.204%
49	21.127	3080	3084	3091	rVB2	812601	1169950	4.49%	0.479%
50	21.262	3105	3107	3110	rVB2	478939	464800	1.78%	0.190%
51	21.339	3111	3120	3125	rBV3	8411006	18204044	69.87%	7.447%
52	21.386	3125	3128	3137	rVB	5560483	7141432	27.41%	2.921%
53	21.468	3137	3142	3146	rBV	4539350	6165641	23.66%	2.522%
54	21.509	3146	3149	3154	rVB	1238836	1712268	6.57%	0.700%
55	21.674	3173	3177	3182	rBV2	793356	1143317	4.39%	0.468%
56	23.039	3402	3409	3414	rBV	4291150	10941314	41.99%	4.476%
57	23.221	3436	3440	3446	rVB	755012	1260413	4.84%	0.516%
58	23.562	3492	3498	3507	rVB	2350277	4945765	18.98%	2.023%
59	23.668	3509	3516	3524	rVB	3565485	7439843	28.55%	3.043%
60	23.774	3527	3534	3539	rBV2	3111382	6844433	26.27%	2.800%
61	26.297	3955	3963	3977	rVB2	1822667	5839014	22.41%	2.389%

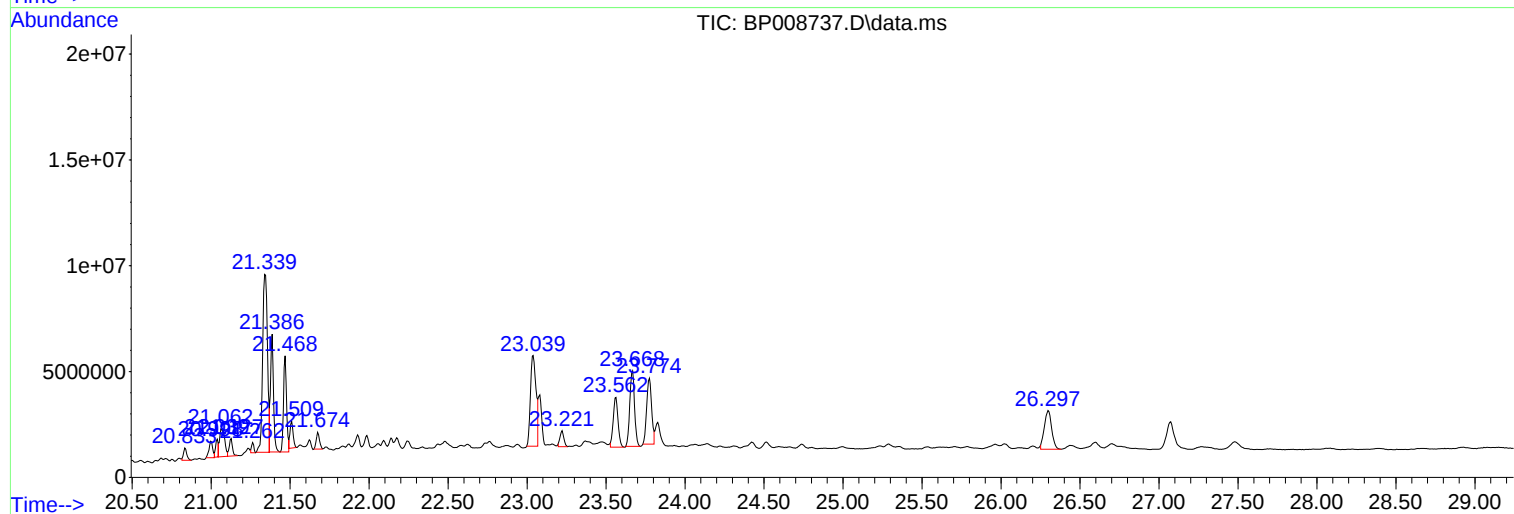
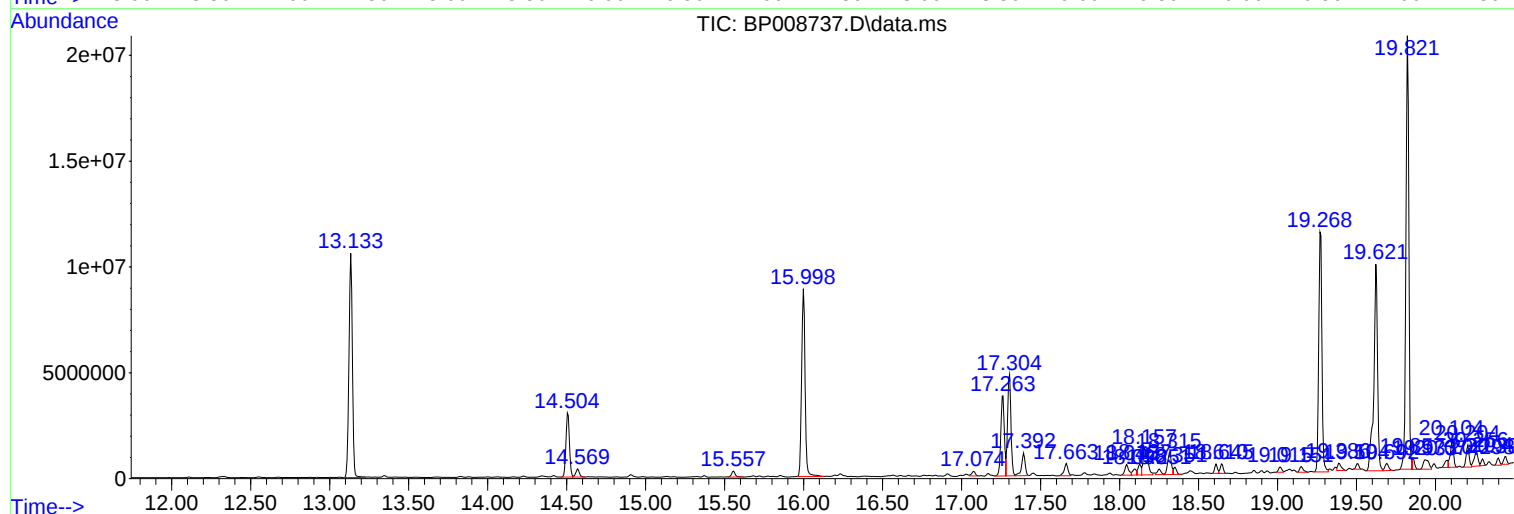
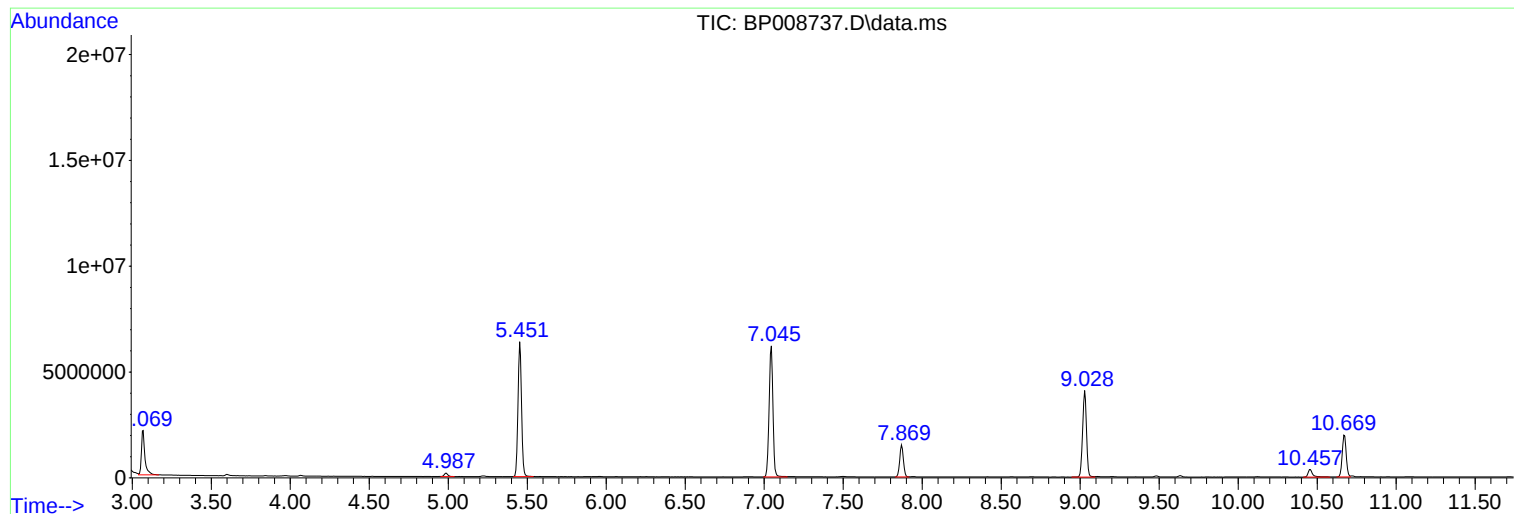
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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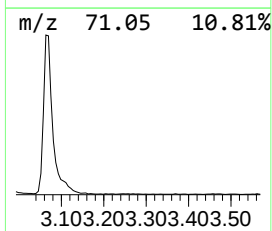
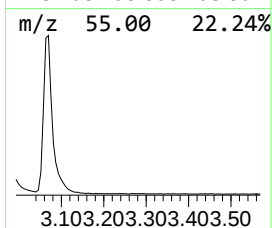
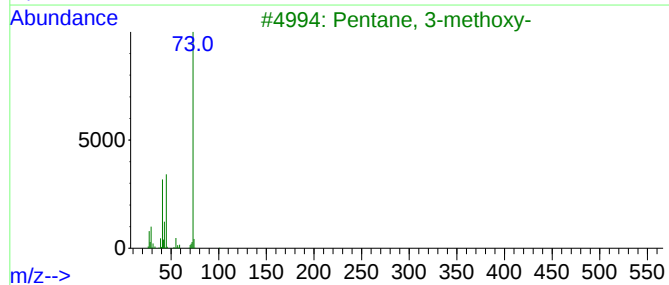
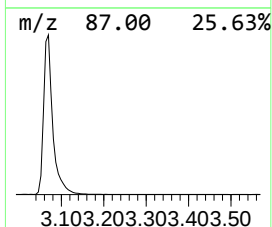
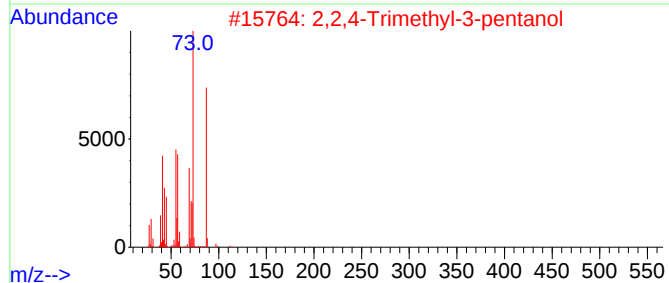
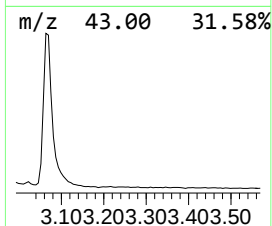
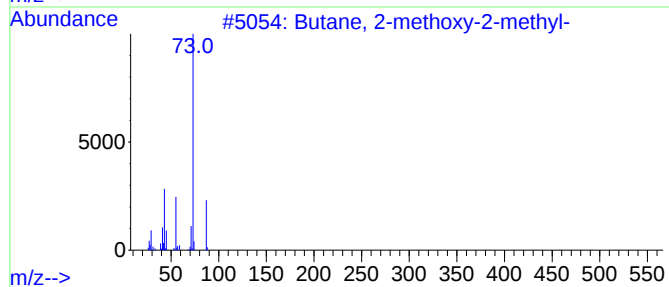
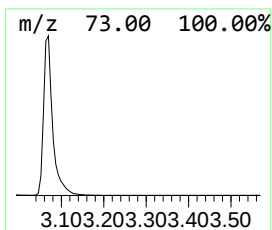
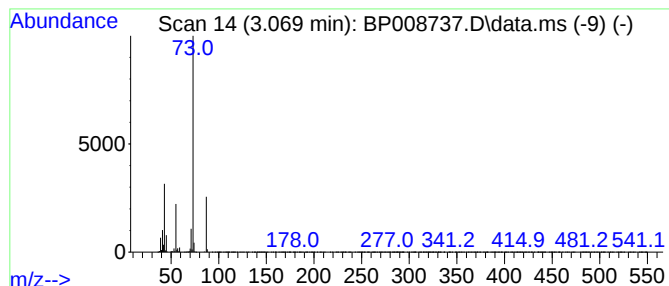
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.069	26.67 ng	3230830	1,4-Dichlorobenzene-d4	7.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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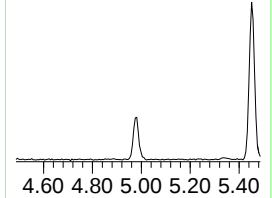
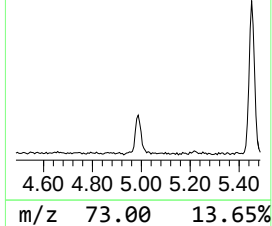
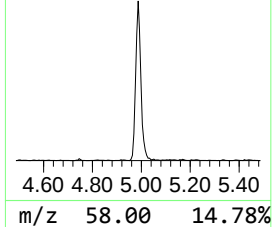
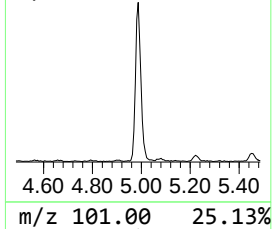
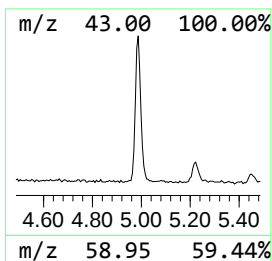
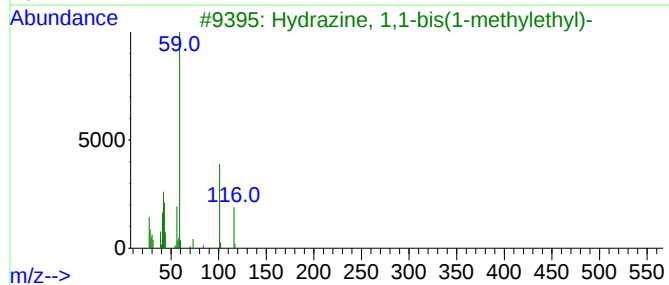
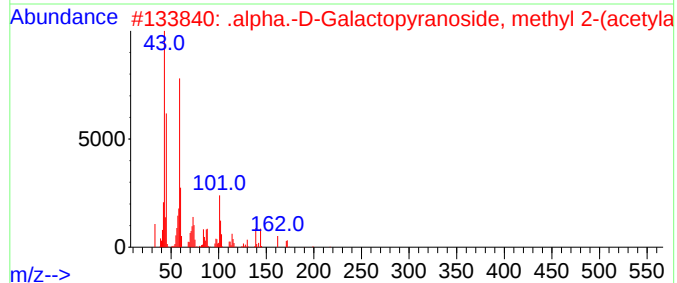
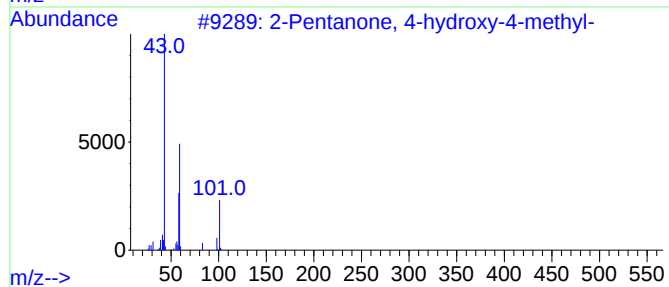
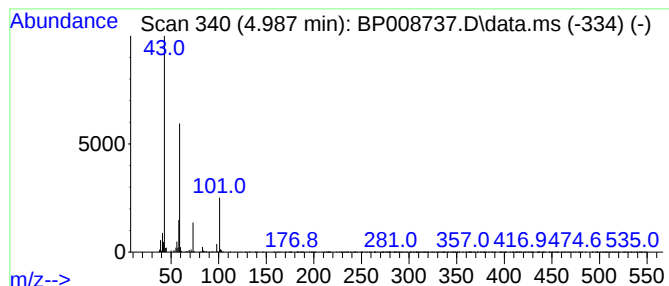
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.987	2.23 ng	270495	1,4-Dichlorobenzene-d4			7.869
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	.alpha.-D-Galactopyranoside, met...		249	C10H19NO6	017296-07-0	39
3	Hydrazine, 1,1-bis(1-methylethyl)-		116	C6H16N2	000921-14-2	25
4	3-Pentanol		88	C5H12O	000584-02-1	23
5	Butane, 1-ethoxy-		102	C6H14O	000628-81-9	23



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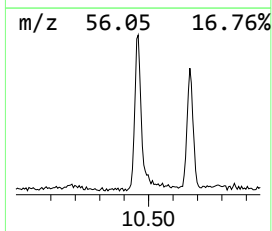
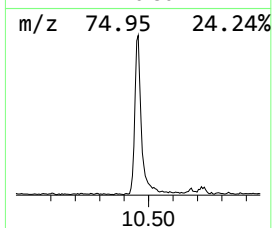
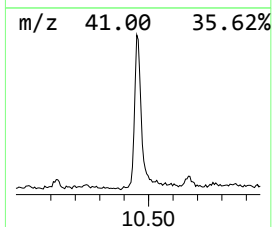
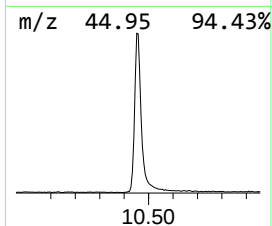
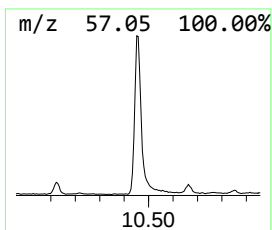
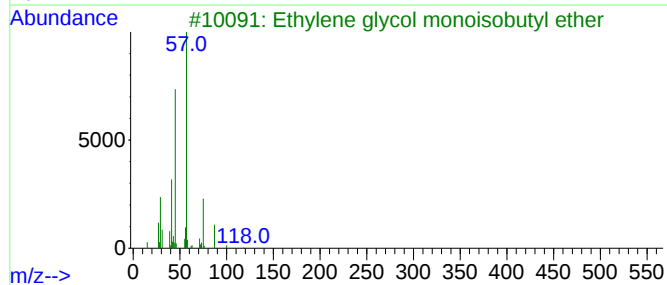
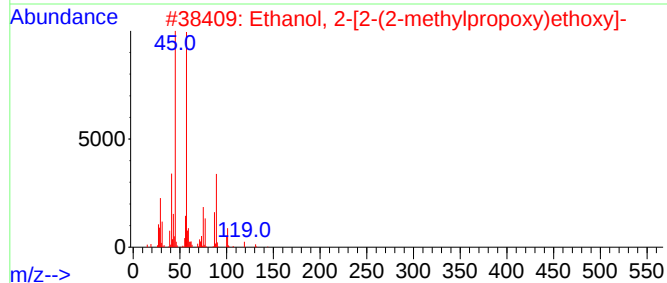
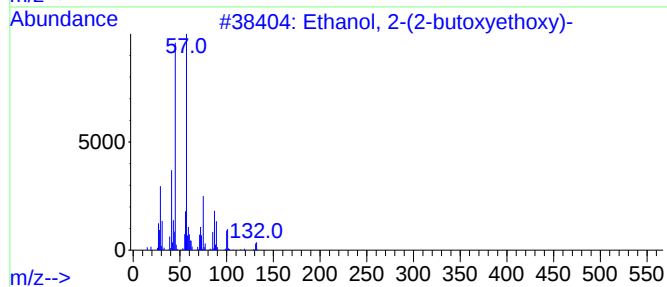
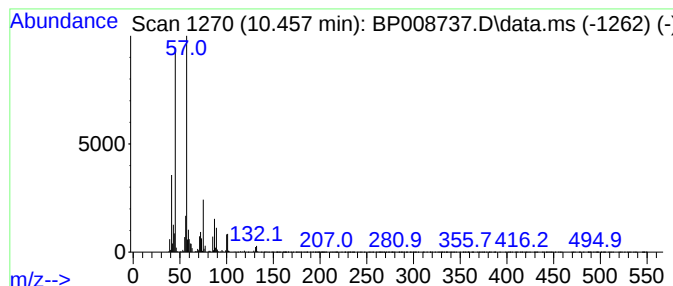
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.457	4.22 ng	729248	Naphthalene-d8	10.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	59
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	52



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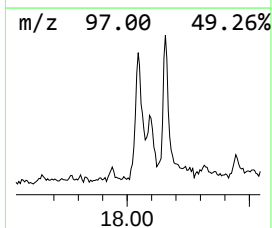
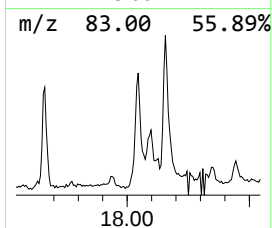
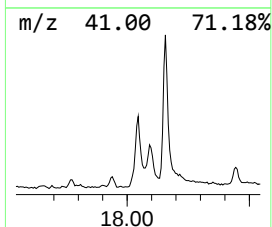
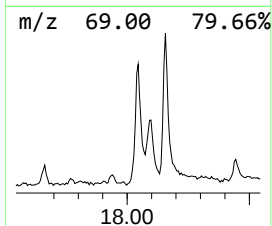
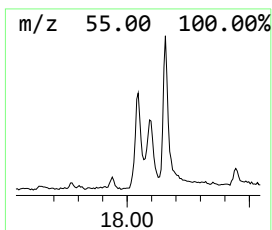
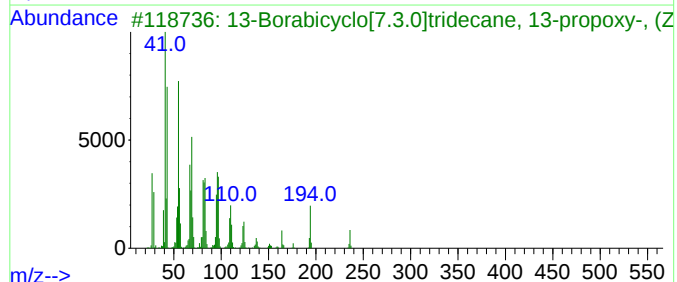
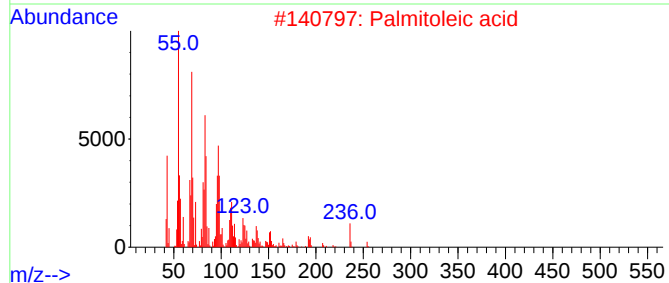
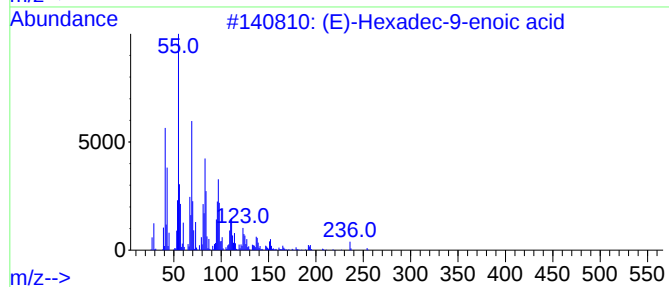
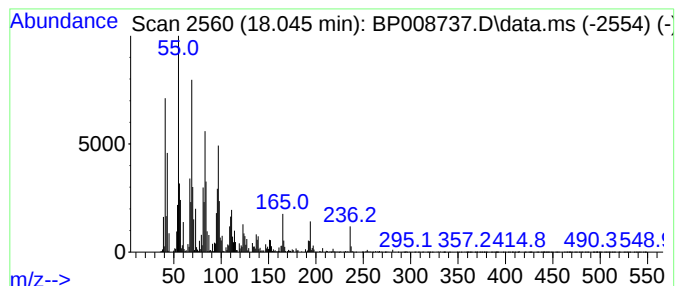
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (E)-Hexadec-9-enoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.045	2.91 ng	876731	Phenanthrene-d10	17.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	97		
2	Palmitoleic acid	254	C16H30O2	000373-49-9	94		
3	13-Borabicyclo[7.3.0]tridecane, ...	236	C15H29BO	1000156-41-7	91		
4	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	83		
5	1-Cyclohexyl-2-methyl-prop-2-en-...	152	C10H16O	025183-82-8	78		



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Acq On : 07 Jan 2022 21:15
Operator : CG/JU
Sample : N1069-02
Misc :
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ClientSampleId :
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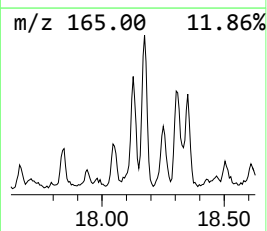
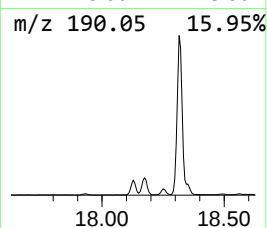
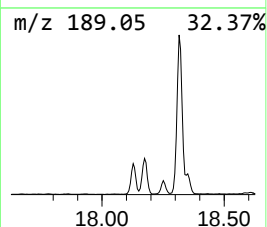
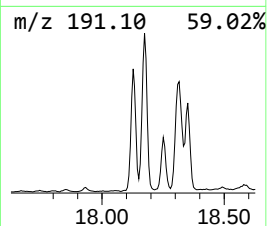
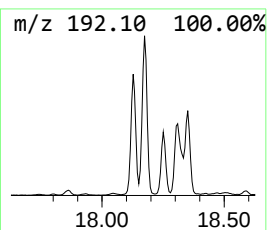
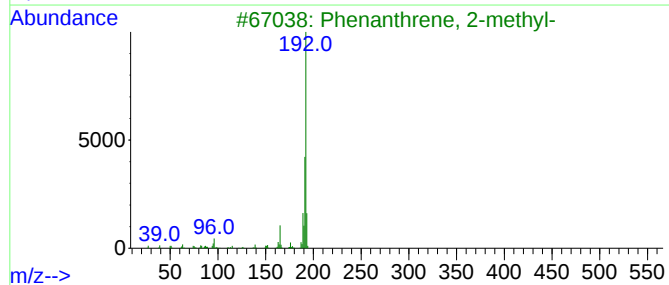
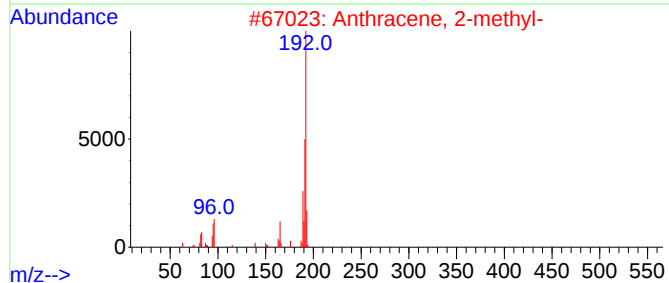
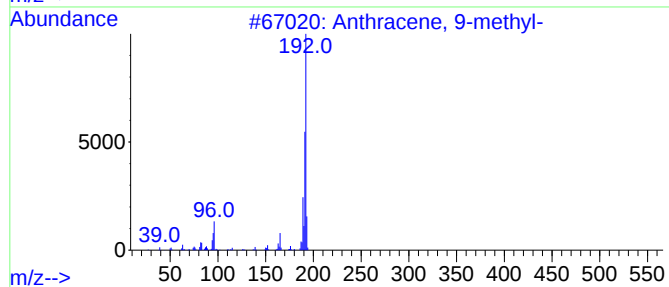
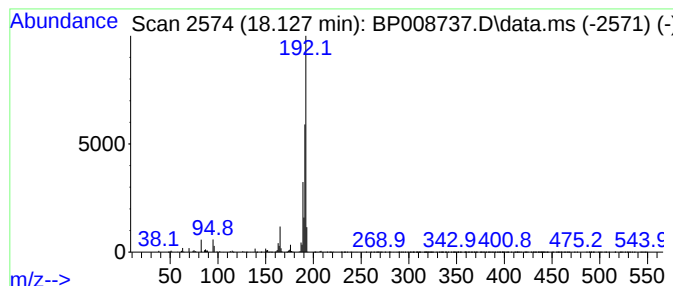
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Anthracene, 9-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.127	2.31 ng	696409	Phenanthrene-d10	17.262

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	81
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	76
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	76
5			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008737.D
Acq On : 07 Jan 2022 21:15
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Misc :
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Instrument :
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ClientSampleId :
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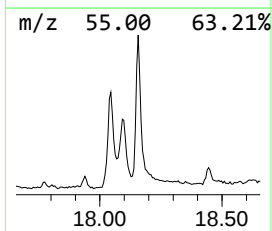
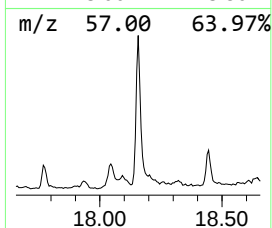
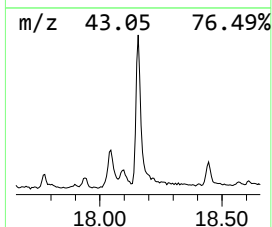
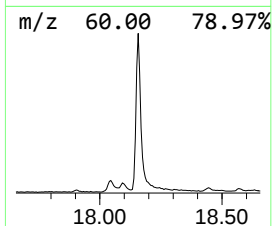
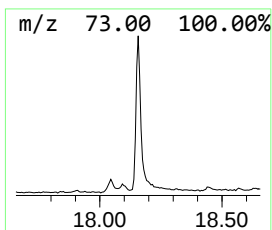
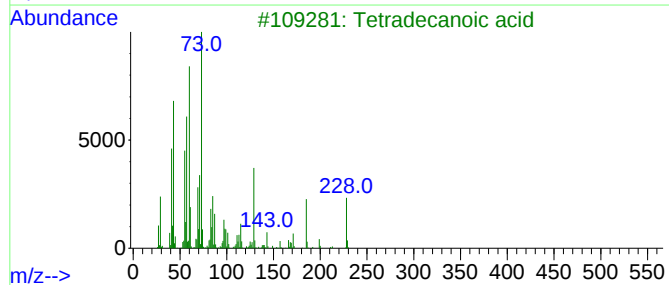
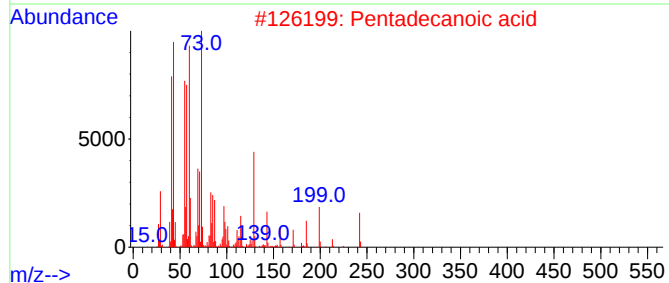
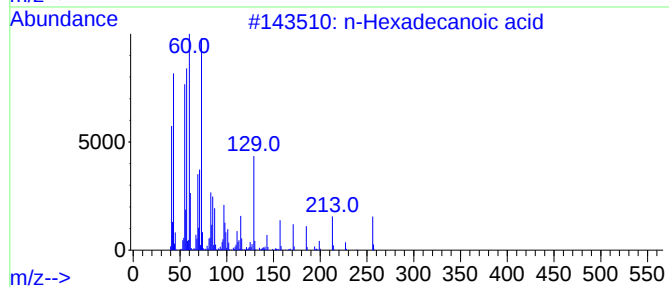
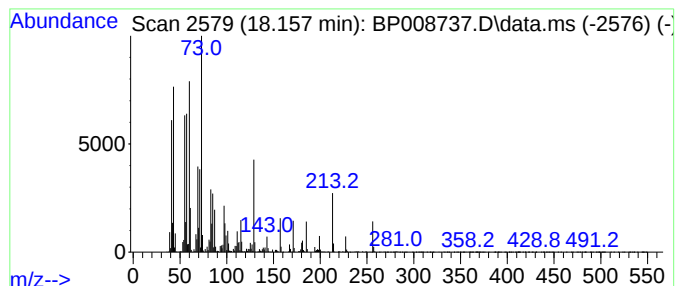
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	8.67 ng	2613570	Phenanthrene-d10	17.262

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	90
5		Undecanoic acid	186	C11H22O2	000112-37-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008737.D
Acq On : 07 Jan 2022 21:15
Operator : CG/JU
Sample : N1069-02
Misc :
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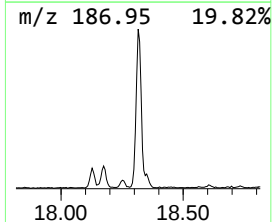
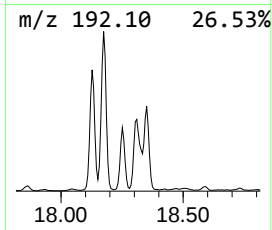
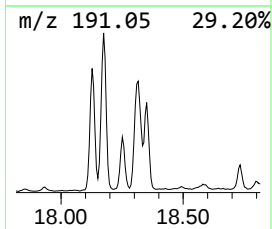
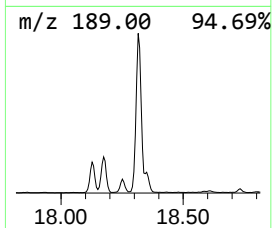
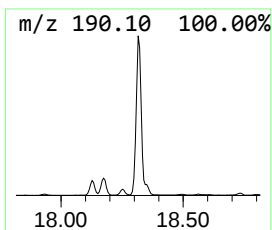
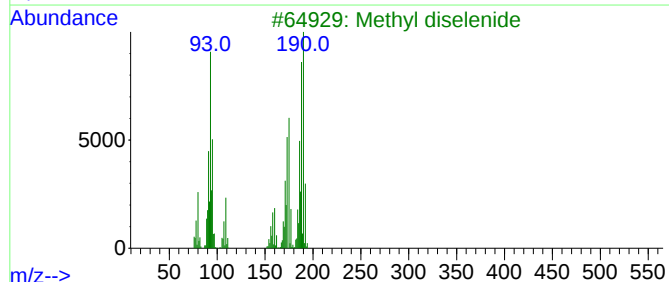
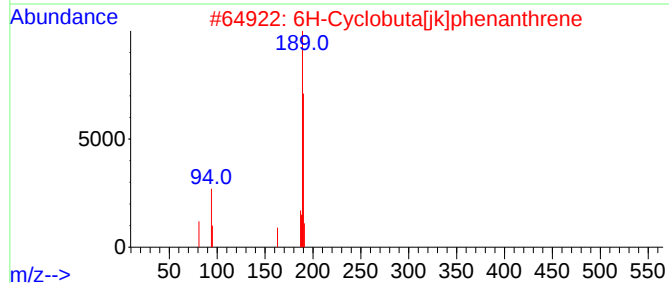
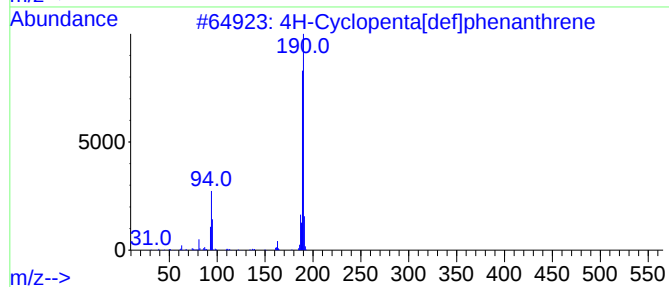
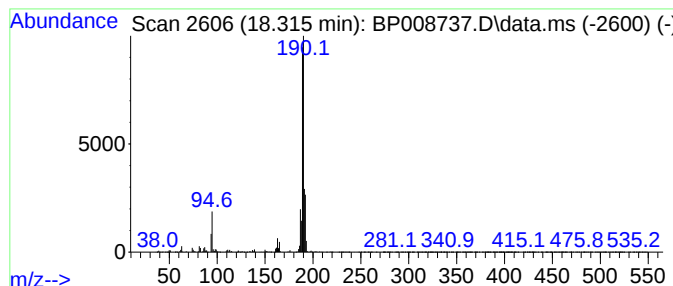
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.315	5.68 ng	1711840	Phenanthrene-d10	17.262	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	64
3	Methyl diselenide	190	C2H6Se2	007101-31-7	55
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008737.D
Acq On : 07 Jan 2022 21:15
Operator : CG/JU
Sample : N1069-02
Misc :
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Instrument :
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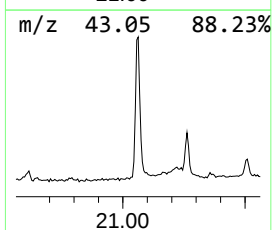
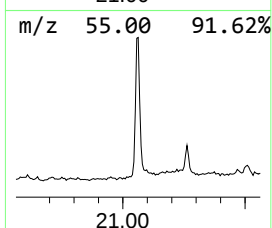
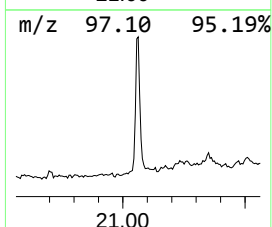
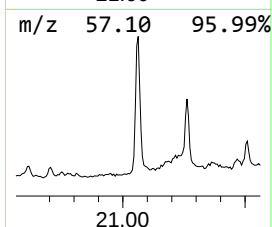
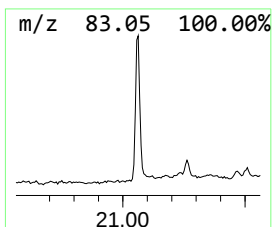
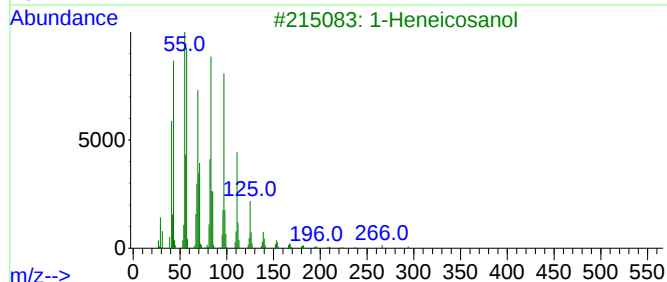
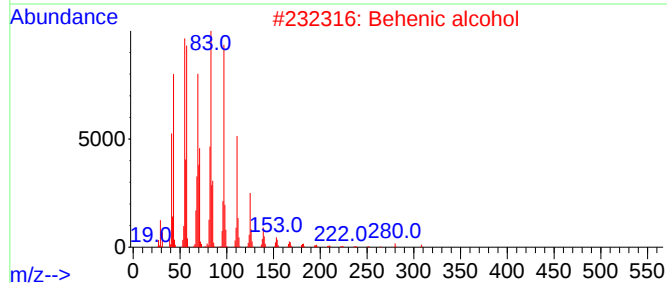
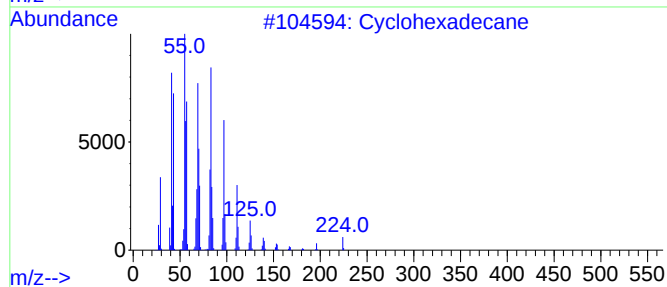
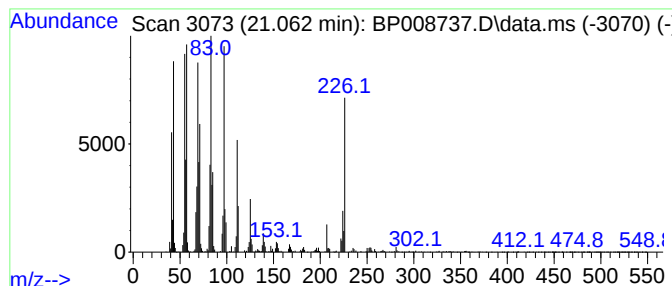
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.062	3.23 ng	2943560	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	94
2			Behenic alcohol	326	C22H46O	000661-19-8	90
3			1-Heneicosanol	312	C21H44O	015594-90-8	90
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008737.D
Acq On : 07 Jan 2022 21:15
Operator : CG/JU
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Misc :
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Instrument :
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ClientSampleId :
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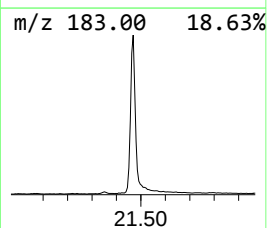
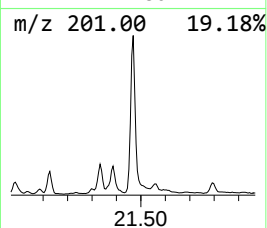
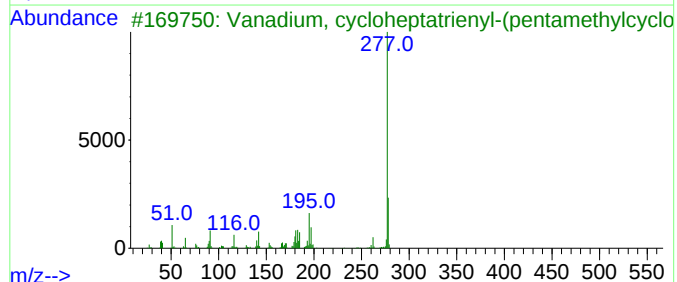
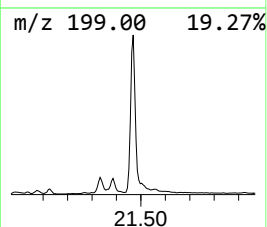
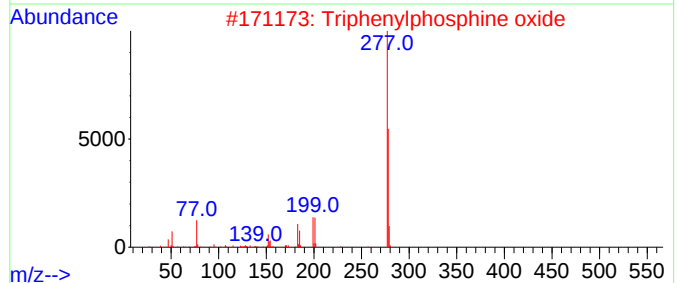
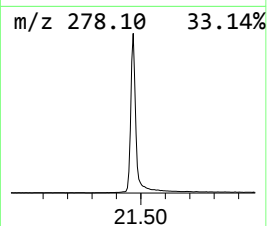
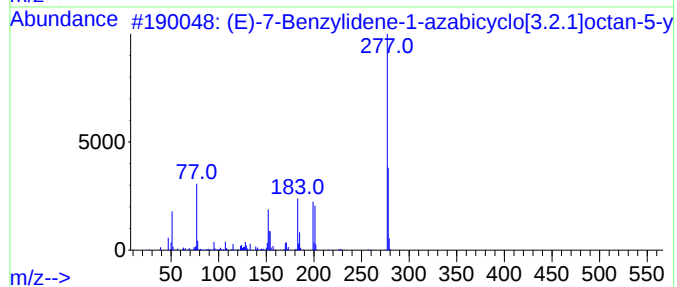
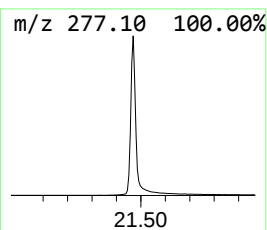
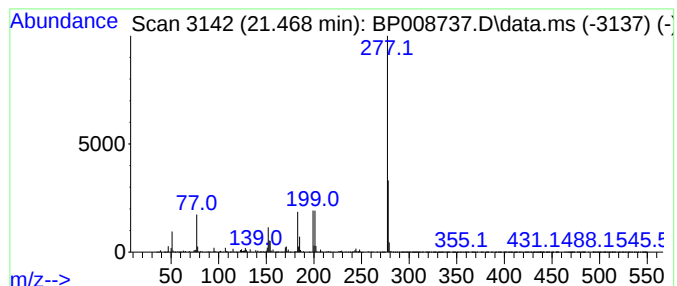
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 (E)-7-Benzylidene-1-azabicy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.468	6.77 ng	6165640	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	86		
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	72		
3	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	50		
4	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32		
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
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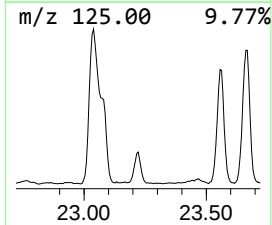
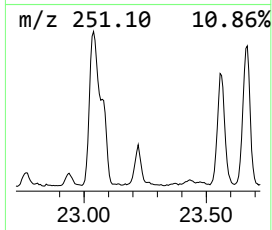
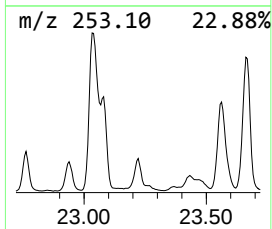
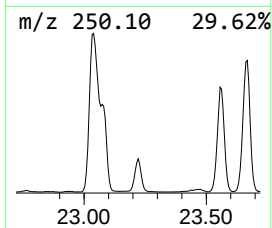
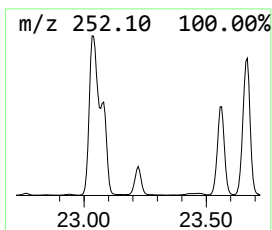
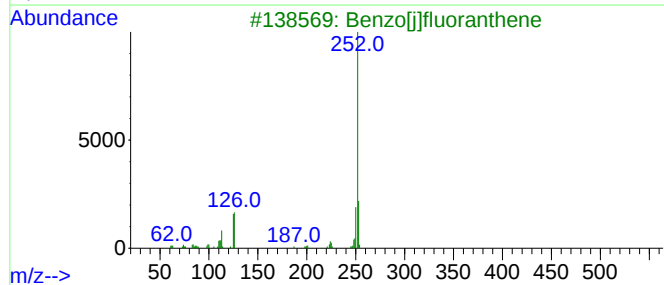
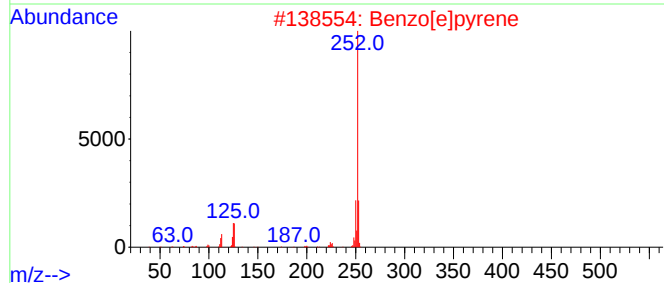
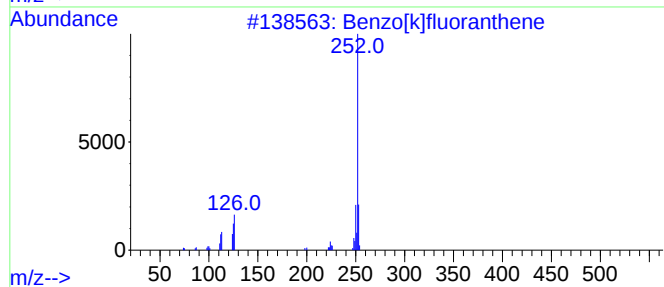
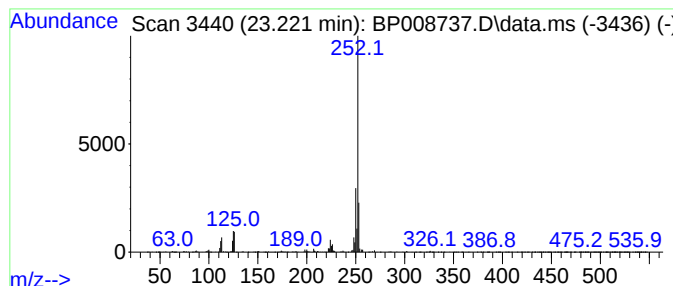
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.221	3.68 ng	1260410	Perylene-d12	23.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2			Benzo[e]pyrene	252	C20H12	000192-97-2	95
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4			Perylene	252	C20H12	000198-55-0	90
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008737.D
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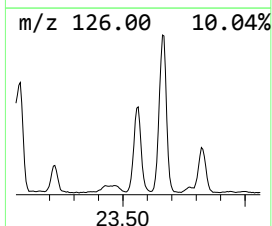
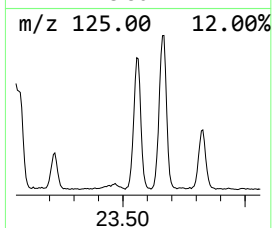
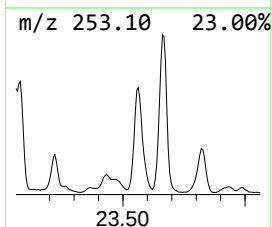
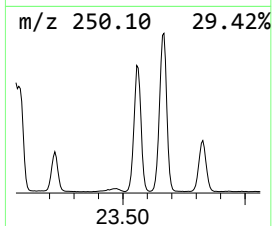
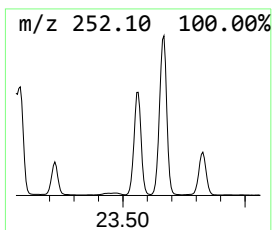
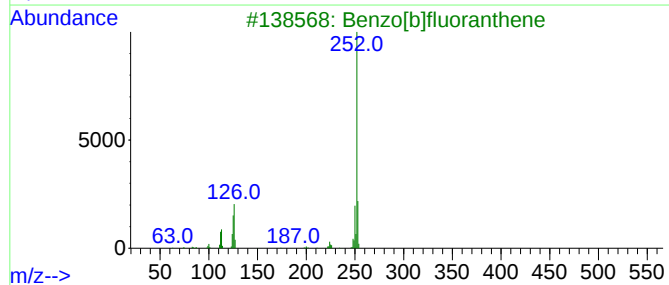
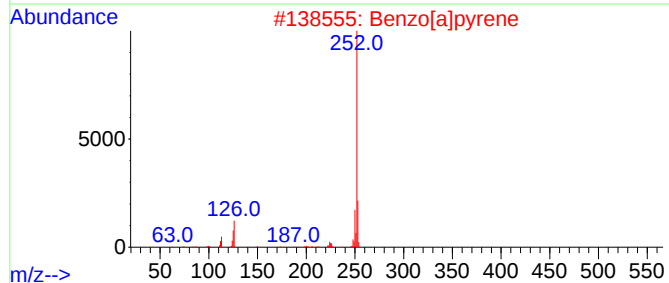
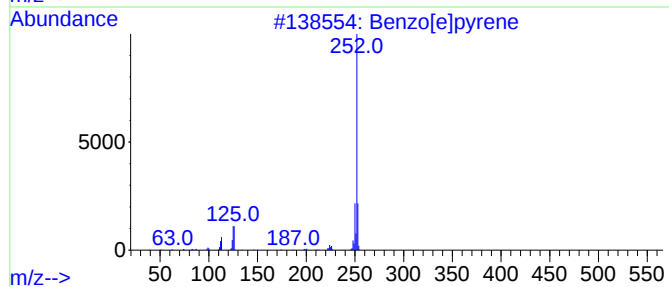
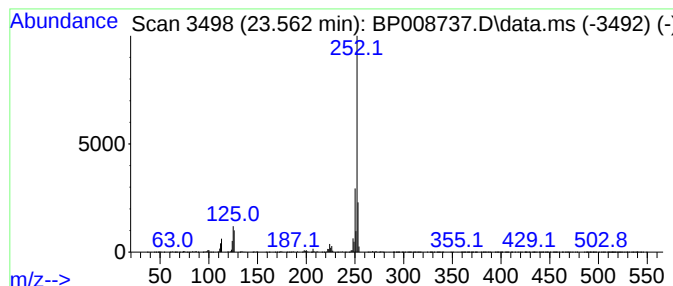
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.562	14.45 ng	4945770	Perylene-d12	23.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	99
2		Benzo[a]pyrene	252	C20H12	000050-32-8	97
3		Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4		Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5		Perylene	252	C20H12	000198-55-0	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010722\
Data File : BP008737.D
Acq On : 07 Jan 2022 21:15
Operator : CG/JU
Sample : N1069-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PX-2-010522

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP010622.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
Butane, 2-metho...	3.069	26.7	ng	3230830	1	7.869	2422490	20.0
2-Pentanone, 4-...	4.987	2.2	ng	270495	1	7.869	2422490	20.0
Ethanol, 2-(2-b...	10.457	4.2	ng	729248	2	10.669	3459390	20.0
(E)-Hexadec-9-e...	18.045	2.9	ng	876731	4	17.262	6026990	20.0
Anthracene, 9-m...	18.127	2.3	ng	696409	4	17.262	6026990	20.0
n-Hexadecanoic ...	18.157	8.7	ng	2613570	4	17.262	6026990	20.0
4H-Cyclopenta[d...	18.315	5.7	ng	1711840	4	17.262	6026990	20.0
Cyclohexadecane	21.062	3.2	ng	2943560	5	21.351	18204000	20.0
(E)-7-Benzylide...	21.468	6.8	ng	6165640	5	21.351	18204000	20.0
Benzo[e]pyrene	23.221	3.7	ng	1260410	6	23.774	6844430	20.0
Perylene	23.562	14.4	ng	4945770	6	23.774	6844430	20.0