

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
 Data File : BP005370.D
 Acq On : 22 Apr 2021 12:01
 Operator : CG/JU
 Sample : M2024-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 FK-GF-02-071-B

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-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005370.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	360	367	387	rBV	678491	975454	42.97%	7.560%
2	6.828	627	636	653	rBV	615983	1035490	45.61%	8.025%
3	7.640	766	774	784	rBV	159862	246581	10.86%	1.911%
4	8.804	965	972	989	rBV	389020	642977	28.32%	4.983%
5	10.428	1240	1248	1254	rBV	172702	304689	13.42%	2.361%
6	12.916	1661	1671	1681	rBV	896464	1254106	55.24%	9.720%
7	13.769	1810	1816	1824	rBV	17645	32043	1.41%	0.248%
8	14.304	1898	1907	1913	rBV	270972	398779	17.56%	3.091%
9	15.363	2081	2087	2096	rVB2	17121	27973	1.23%	0.217%
10	15.804	2155	2162	2172	rBV	840035	1193455	52.57%	9.250%
11	17.063	2371	2376	2380	rBV	348368	503978	22.20%	3.906%
12	17.110	2380	2384	2391	rVV	169219	245988	10.83%	1.906%
13	17.198	2394	2399	2406	rVB	38786	62136	2.74%	0.482%
14	17.486	2440	2448	2453	rBV	16794	32006	1.41%	0.248%
15	17.945	2520	2526	2527	rBV	29583	40721	1.79%	0.316%
16	17.968	2527	2530	2539	rVB2	107676	183601	8.09%	1.423%
17	18.133	2552	2558	2561	rBV3	42013	70221	3.09%	0.544%
18	18.168	2561	2564	2570	rVB2	19105	28210	1.24%	0.219%
19	18.433	2605	2609	2614	rBV2	26148	40784	1.80%	0.316%
20	18.698	2650	2654	2661	rVB	72630	89511	3.94%	0.694%
21	18.851	2673	2680	2684	rBV4	21784	58372	2.57%	0.452%
22	18.886	2684	2686	2691	rVB5	16426	23051	1.02%	0.179%
23	19.092	2716	2721	2729	rVB	301508	377963	16.65%	2.929%
24	19.209	2735	2741	2744	rBV5	51589	77252	3.40%	0.599%
25	19.315	2756	2759	2764	rVB2	19496	28677	1.26%	0.222%
26	19.445	2772	2781	2789	rBV	236381	364837	16.07%	2.828%
27	19.645	2809	2815	2821	rBV	1974155	2270338	100.00%	17.596%
28	19.762	2831	2835	2841	rBV4	19233	41757	1.84%	0.324%
29	19.927	2860	2863	2869	rVB	42829	64548	2.84%	0.500%
30	20.027	2877	2880	2885	rBV2	32549	45530	2.01%	0.353%
31	20.086	2887	2890	2893	rVB2	19935	27660	1.22%	0.214%
32	20.304	2924	2927	2933	rVB	32621	45087	1.99%	0.349%
33	20.509	2958	2962	2965	rBV	101344	109354	4.82%	0.848%
34	20.886	3022	3026	3034	rVB3	138172	215905	9.51%	1.673%
35	21.168	3068	3074	3078	rBV2	627166	894790	39.41%	6.935%
36	21.204	3078	3080	3085	rVB	134211	141143	6.22%	1.094%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.745	3339	3342	3346	rBV	50446	77472	3.41%	0.600%
38	23.427	3452	3458	3464	rBV2	338406	630426	27.77%	4.886%

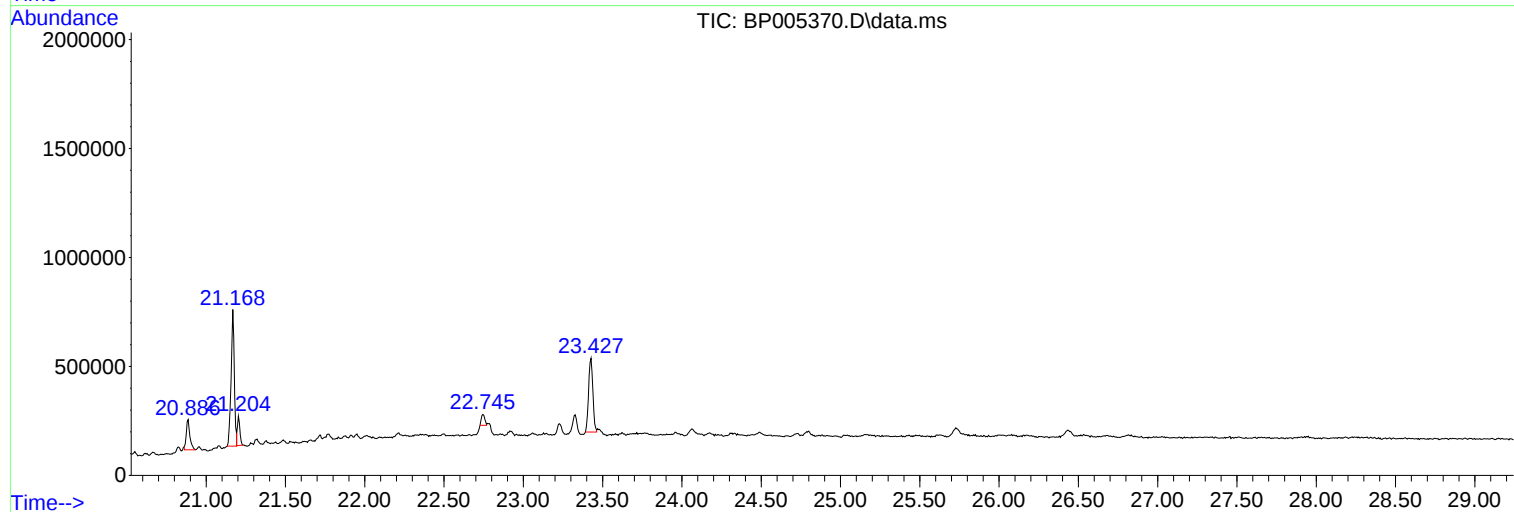
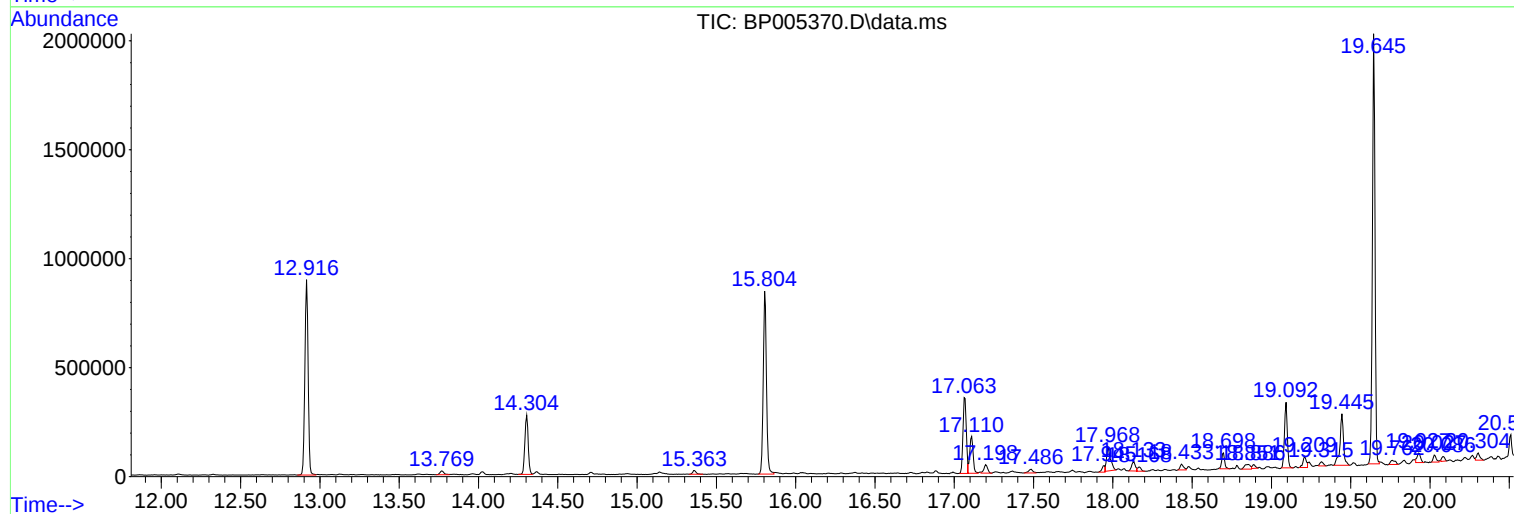
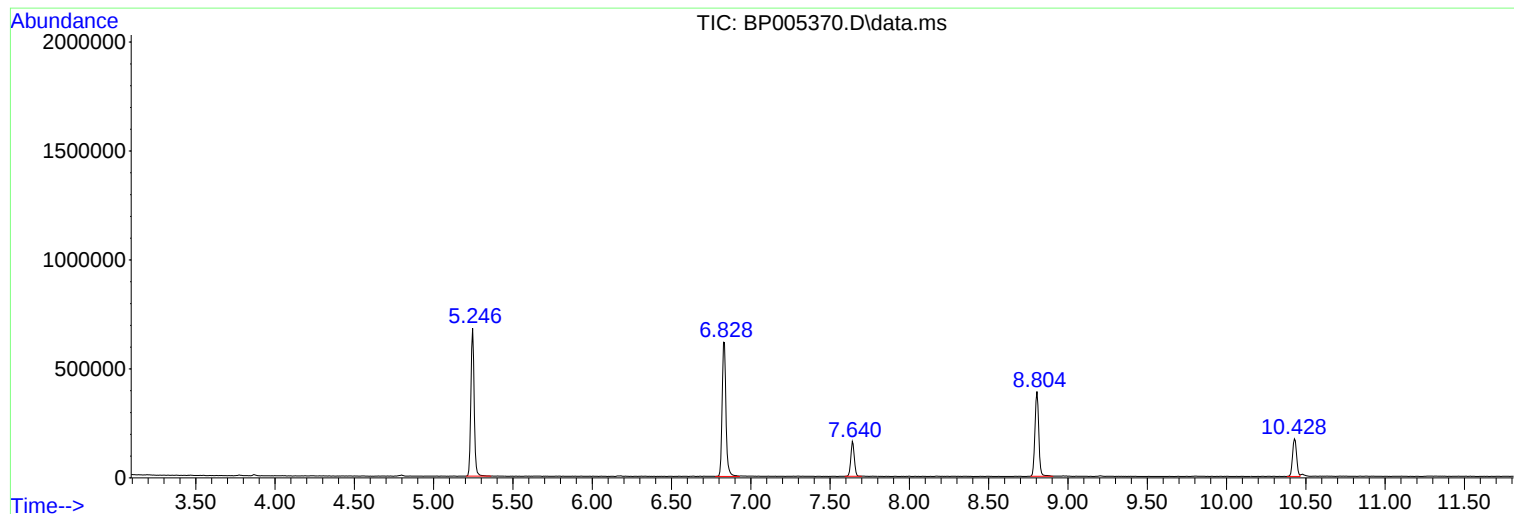
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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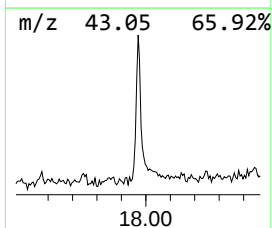
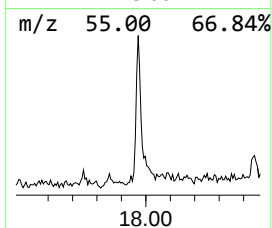
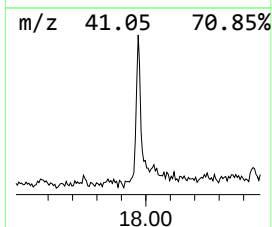
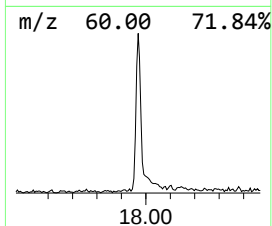
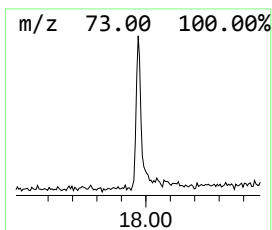
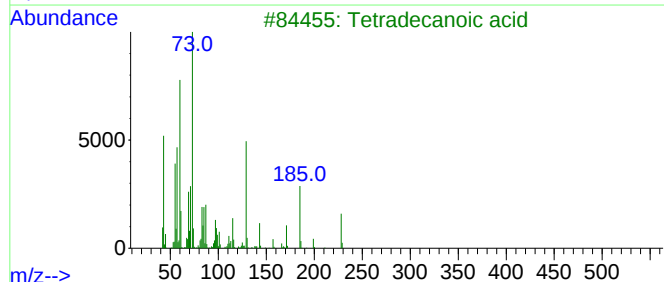
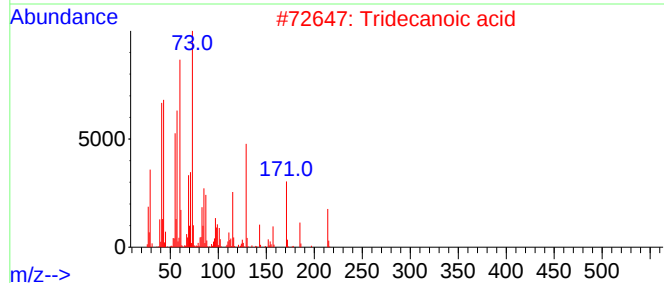
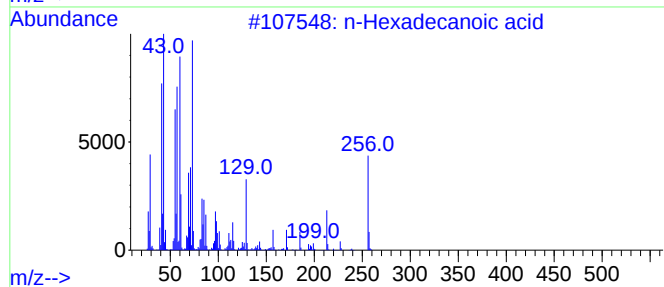
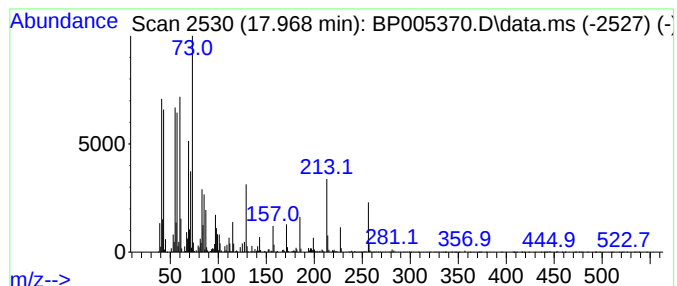
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.968	7.29 ng	183601	Phenanthrene-d10	17.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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ALS Vial : 6 Sample Multiplier: 1

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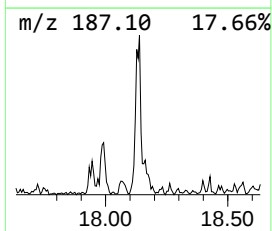
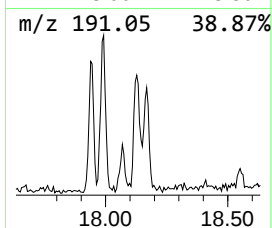
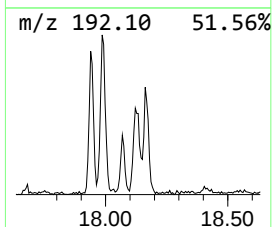
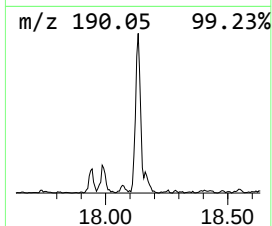
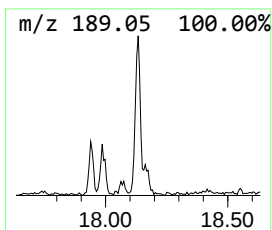
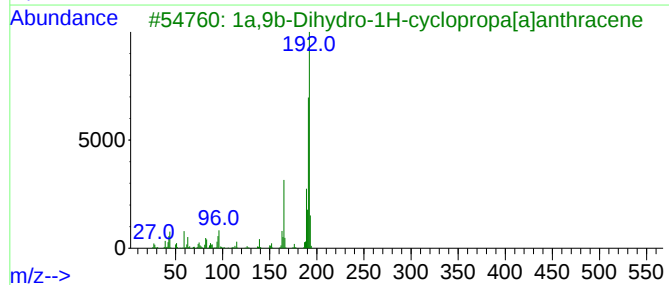
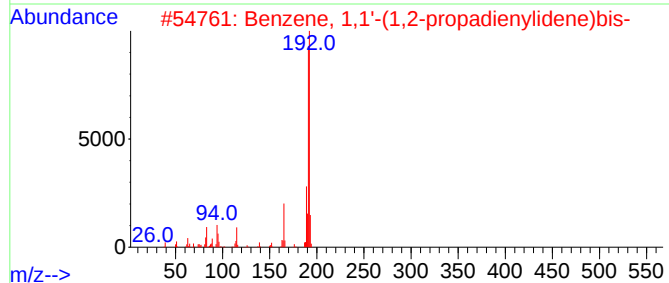
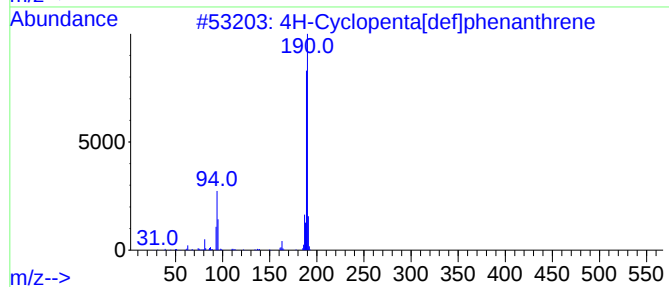
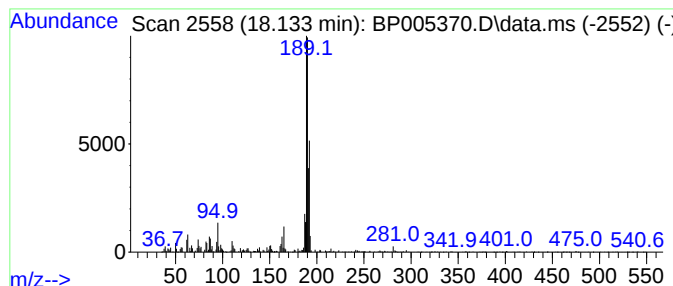
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.133	2.79 ng	70221	Phenanthrene-d10	17.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
2			Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	38
3			1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	30
4			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30
5			Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	25



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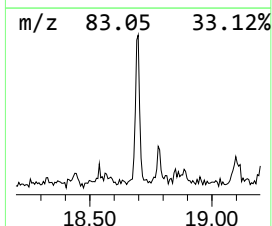
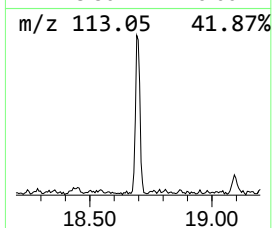
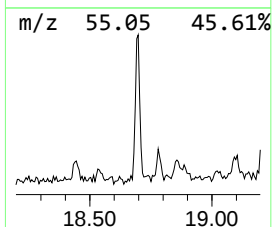
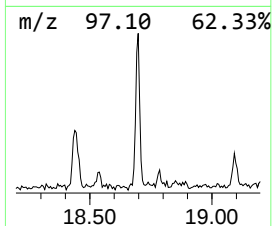
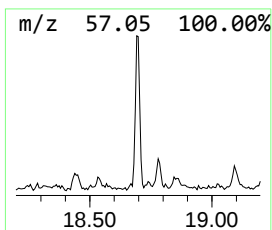
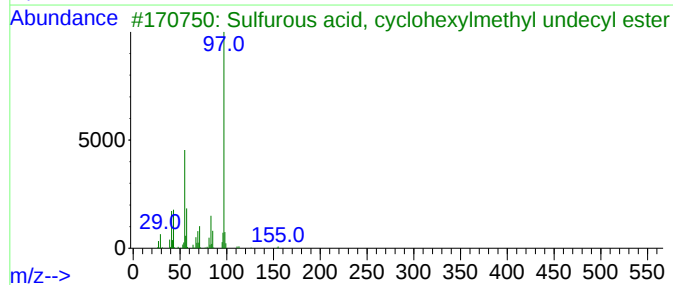
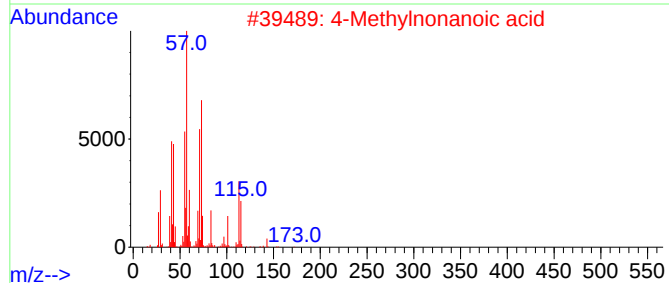
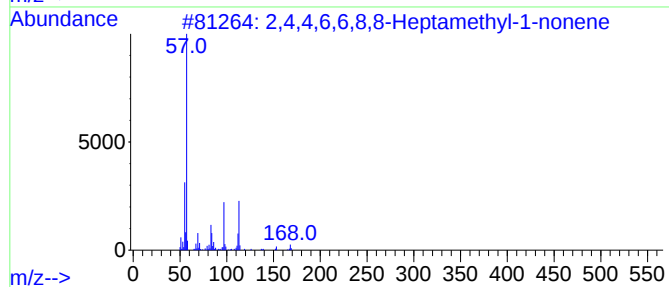
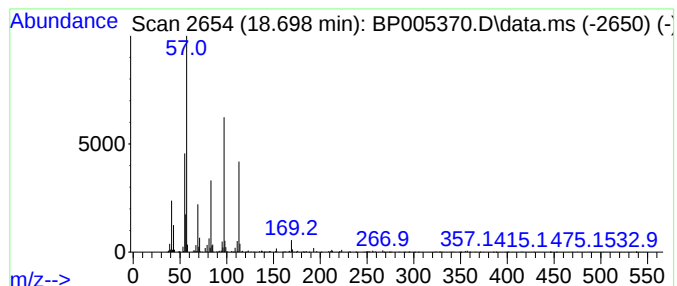
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown18.69 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.698	3.55 ng	89511	Phenanthrene-d10	17.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	40		
2	4-Methylnonanoic acid	172	C10H20O2	045019-28-1	37		
3	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	25		
4	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	25		
5	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	25		



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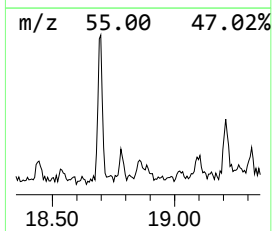
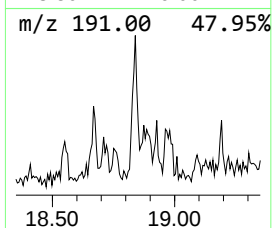
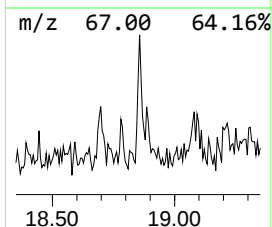
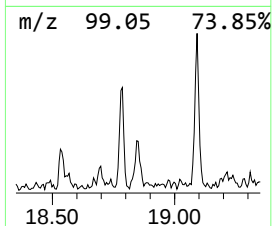
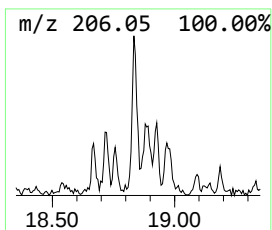
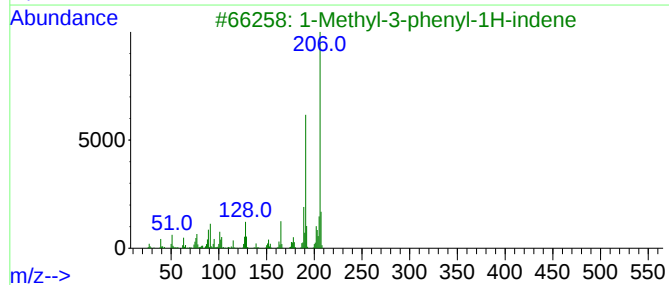
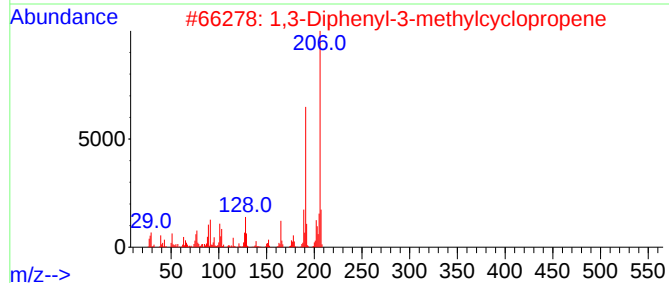
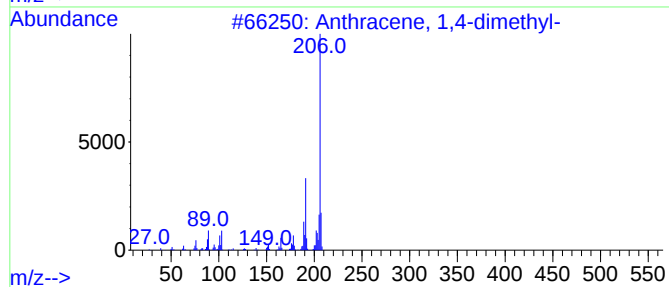
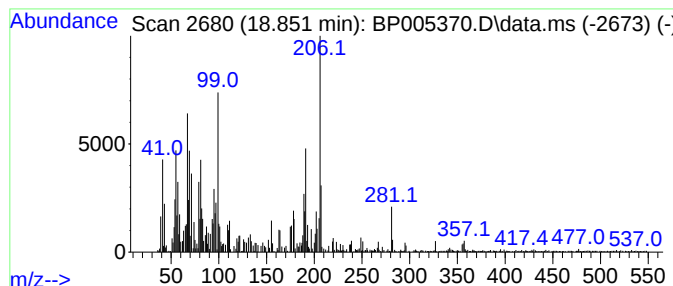
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown18.85 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	2.32 ng	58372	Phenanthrene-d10	17.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	38
2			1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	30
3			1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	30
4			3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	30
5			Scoparone	206	C11H10O4	000120-08-1	30



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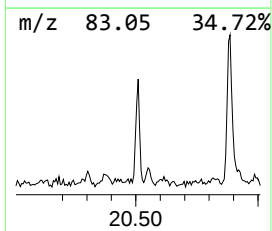
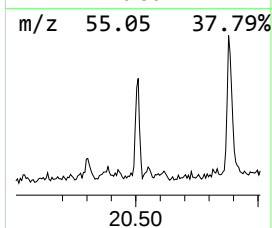
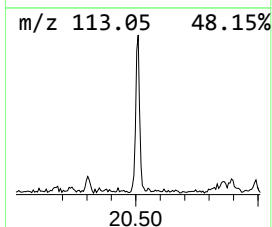
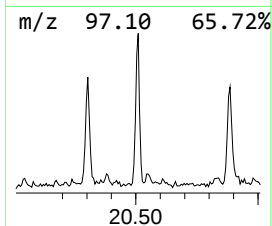
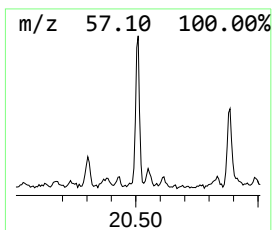
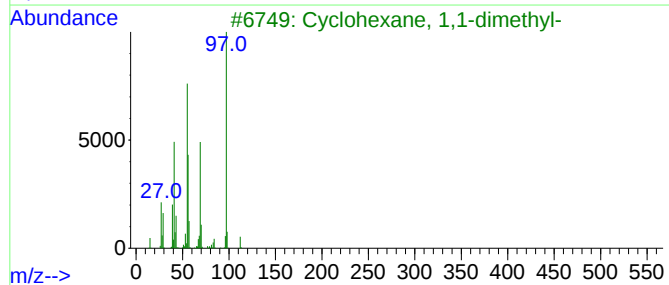
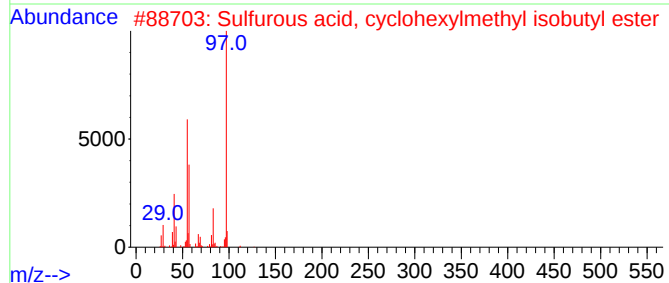
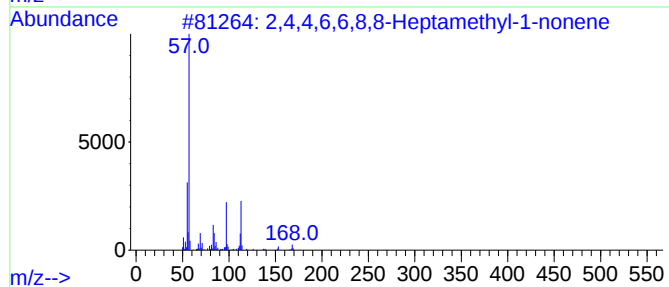
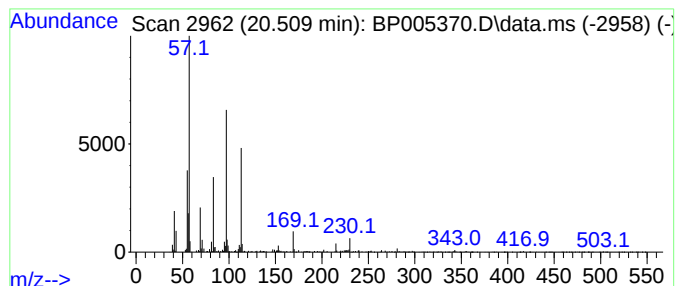
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown20.50 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.509	2.44 ng	109354	Chrysene-d12	21.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	32		
2	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	22		
3	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	18		
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	16		
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	16		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005370.D
Acq On : 22 Apr 2021 12:01
Operator : CG/JU
Sample : M2024-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

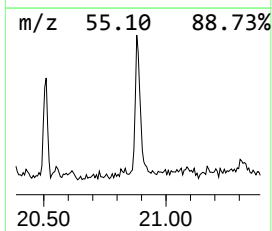
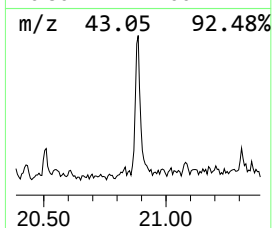
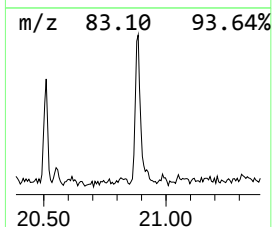
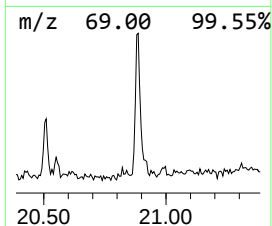
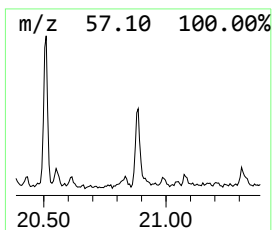
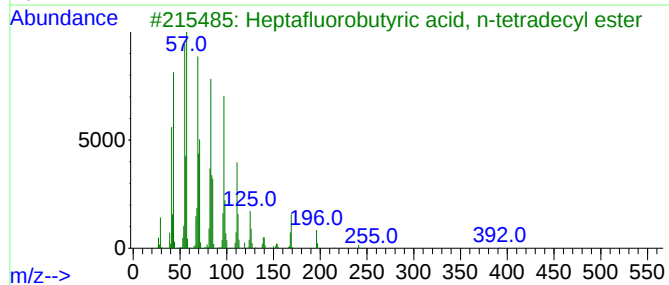
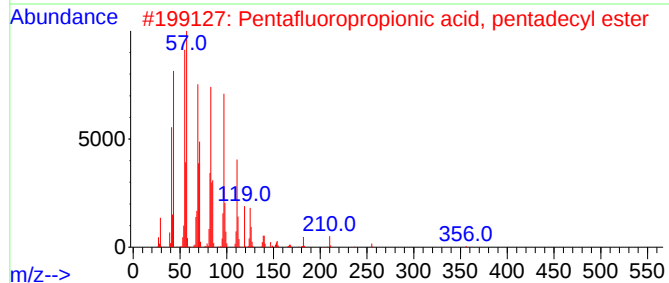
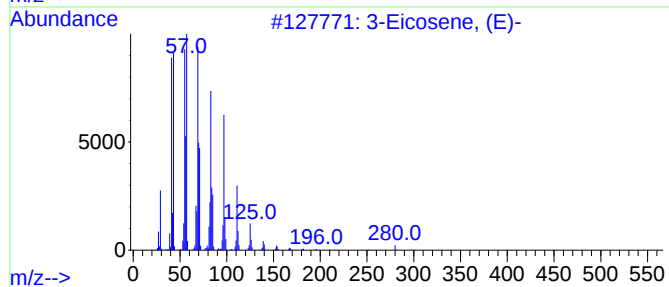
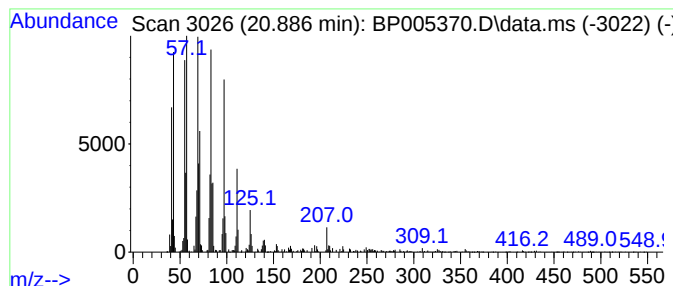
Instrument :
BNA_P
ClientSampleId :
FK-GF-02-071-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.886	4.83 ng	215905	Chrysene-d12	21.168	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	99
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
Data File : BP005370.D
Acq On : 22 Apr 2021 12:01
Operator : CG/JU
Sample : M2024-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FK-GF-02-071-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	17.968	7.3	ng	183601	4	17.068	503978	20.0
4H-Cyclopenta[d]...	18.133	2.8	ng	70221	4	17.068	503978	20.0
unknown18.69	18.698	3.5	ng	89511	4	17.068	503978	20.0
unknown18.85	18.851	2.3	ng	58372	4	17.068	503978	20.0
unknown20.50	20.509	2.4	ng	109354	5	21.168	894790	20.0
3-Eicosene, (E)-	20.886	4.8	ng	215905	5	21.168	894790	20.0