

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
 Data File : BG053537.D
 Acq On : 13 May 2022 11:05
 Operator : CG/JU
 Sample : N2749-19
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-7

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053537.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.649	378	385	395	rBV	395624	664285	34.89%	5.914%
2	7.247	650	657	669	rBV	438692	760261	39.93%	6.769%
3	8.081	791	799	806	rBV	86760	151473	7.96%	1.349%
4	9.244	989	997	1007	rBV	267760	488019	25.63%	4.345%
5	10.895	1271	1278	1284	rBV	114871	205447	10.79%	1.829%
6	13.333	1686	1693	1699	rVB	660611	1043883	54.82%	9.294%
7	14.707	1920	1927	1933	rBV	185496	286130	15.03%	2.547%
8	16.193	2174	2180	2190	rBV	590698	934171	49.06%	8.317%
9	17.456	2388	2395	2399	rBV	245349	388407	20.40%	3.458%
10	17.497	2399	2402	2408	rVB	72685	99788	5.24%	0.888%
11	17.586	2410	2417	2422	rBV	19158	37177	1.95%	0.331%
12	17.850	2460	2462	2470	rVB	14983	24488	1.29%	0.218%
13	18.332	2540	2544	2549	rBV2	83116	130722	6.87%	1.164%
14	18.526	2571	2577	2581	rBV6	17078	34610	1.82%	0.308%
15	18.866	2633	2635	2643	rVB7	20451	28575	1.50%	0.254%
16	19.242	2694	2699	2708	rBV7	24110	62376	3.28%	0.555%
17	19.389	2720	2724	2729	rBV8	12151	23447	1.23%	0.209%
18	19.507	2733	2744	2748	rVV	155328	272895	14.33%	2.430%
19	19.565	2750	2754	2756	rVV5	42503	72978	3.83%	0.650%
20	19.601	2756	2760	2774	rVB6	88995	227816	11.96%	2.028%
21	19.830	2795	2799	2801	rBV2	25904	37653	1.98%	0.335%
22	19.865	2801	2805	2814	rVB	132334	205026	10.77%	1.825%
23	19.935	2814	2817	2822	rVB5	13469	21741	1.14%	0.194%
24	20.059	2831	2838	2843	rBV	1451388	1904107	100.00%	16.953%
25	20.112	2843	2847	2854	rVB3	31884	62024	3.26%	0.552%
26	20.352	2886	2888	2893	rVB2	27707	36035	1.89%	0.321%
27	20.458	2902	2906	2909	rBV3	15896	20166	1.06%	0.180%
28	20.858	2969	2974	2980	rVB3	47683	87502	4.60%	0.779%
29	21.122	3015	3019	3023	rBV	24928	33495	1.76%	0.298%
30	21.357	3054	3059	3064	rBV2	85119	137020	7.20%	1.220%
31	21.633	3103	3106	3111	rVB	39000	60070	3.15%	0.535%
32	21.733	3115	3123	3128	rVV2	325573	682925	35.87%	6.080%
33	21.780	3128	3131	3138	rVB	71755	116199	6.10%	1.035%
34	22.150	3190	3194	3201	rVB6	13770	29186	1.53%	0.260%
35	22.479	3246	3250	3251	rBV3	16456	23449	1.23%	0.209%
36	22.749	3292	3296	3300	rBV6	13252	21541	1.13%	0.192%

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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_G\Methods\8270-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.531	3422	3429	3434	rBV4	36940	91108	4.78%	0.811%
38	23.965	3495	3503	3511	rBV2	102954	347936	18.27%	3.098%
39	24.224	3543	3547	3549	rBV3	19149	28161	1.48%	0.251%
40	24.705	3620	3629	3640	rVB	92547	291006	15.28%	2.591%
41	24.852	3647	3654	3666	rVB2	78773	232640	12.22%	2.071%
42	25.005	3671	3680	3690	rBV	182842	552428	29.01%	4.918%
43	26.121	3863	3870	3881	rVB5	29724	109367	5.74%	0.974%
44	28.753	4308	4318	4335	rVB2	38383	164141	8.62%	1.461%

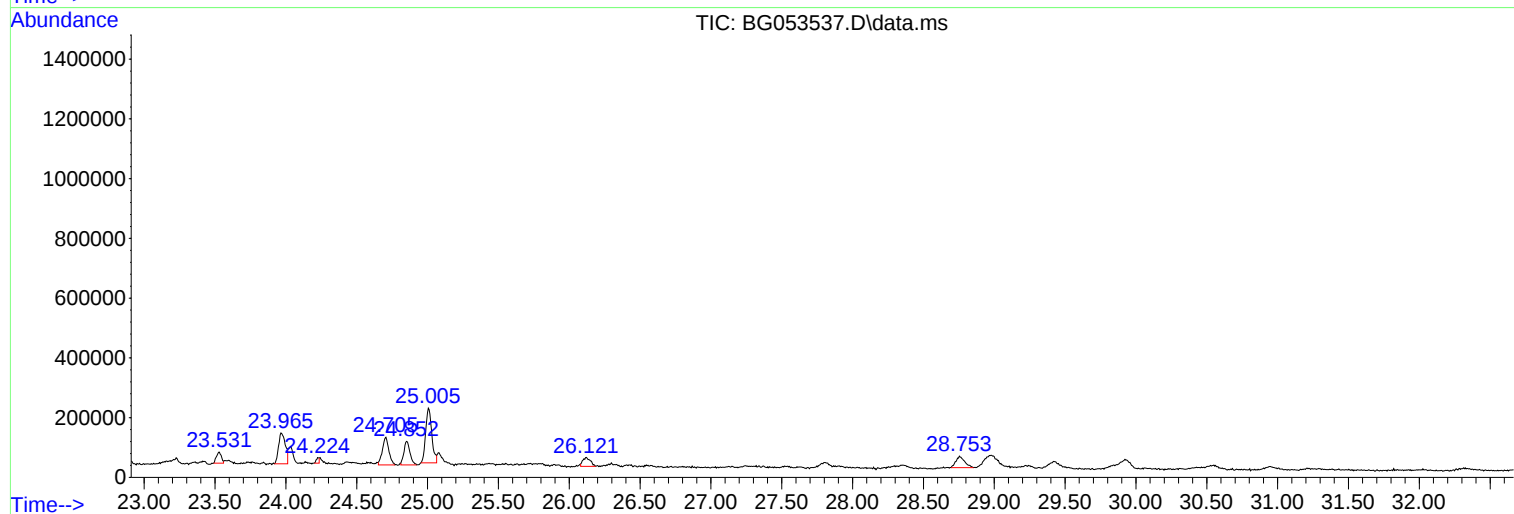
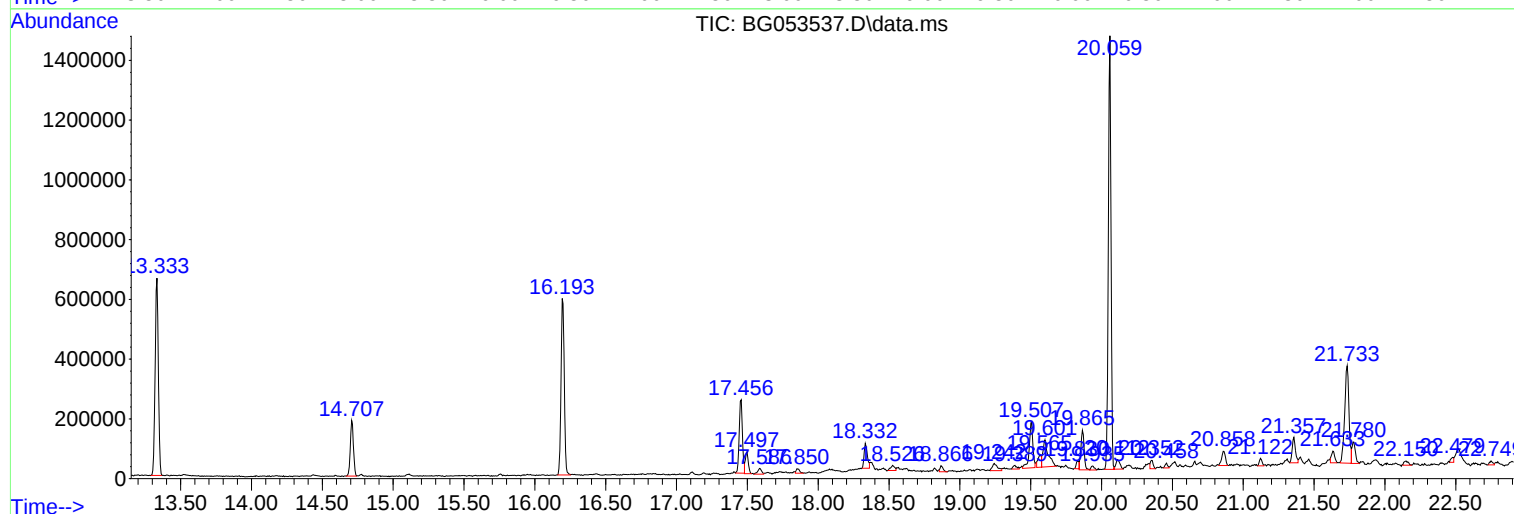
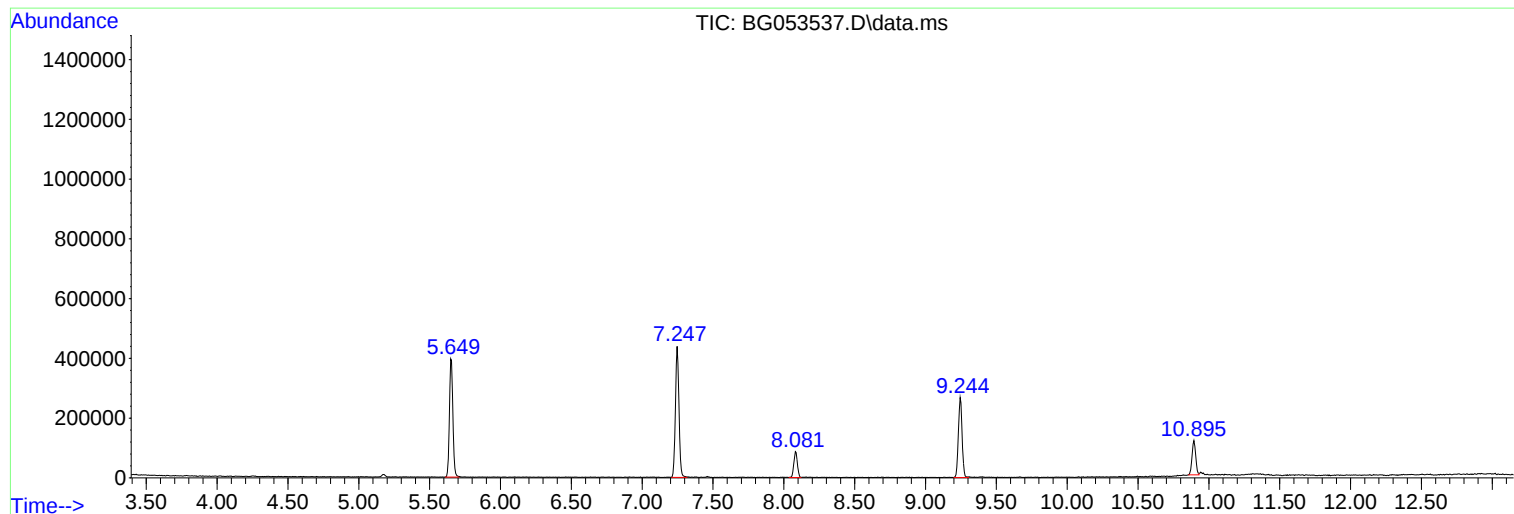
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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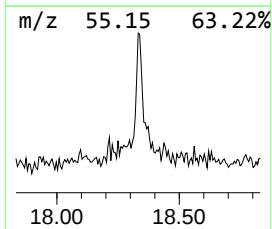
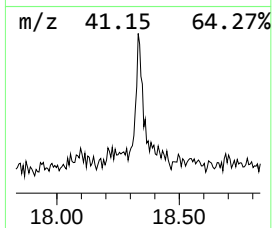
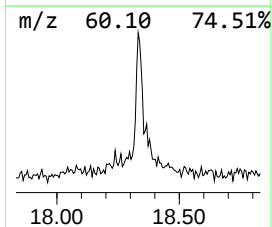
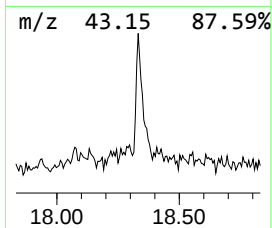
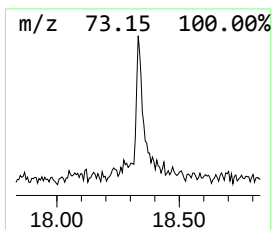
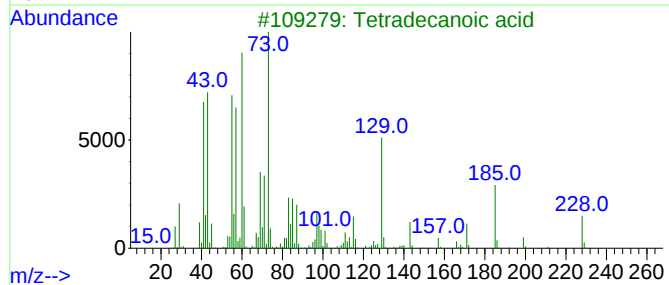
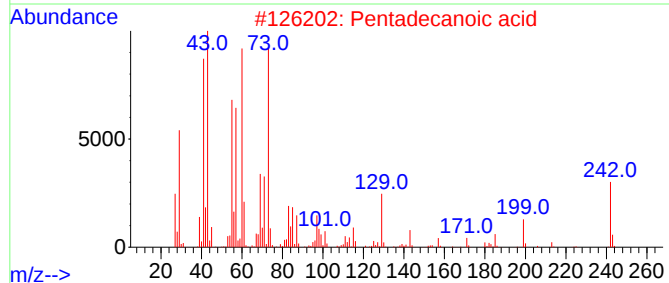
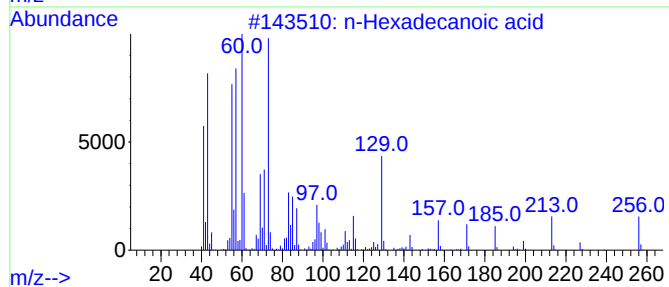
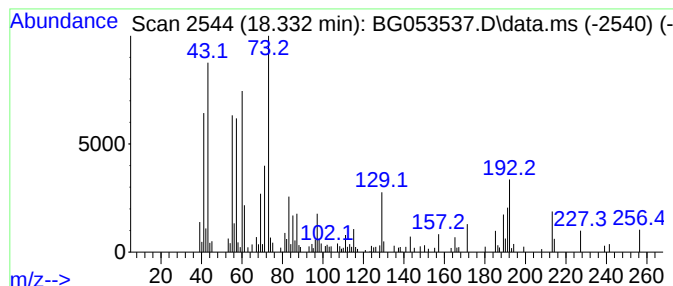
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.332	6.73 ng	130722	Phenanthrene-d10	17.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4			n-Decanoic acid	172	C10H20O2	000334-48-5	42
5			5-Methylhexanoic acid	130	C7H14O2	000628-46-6	37



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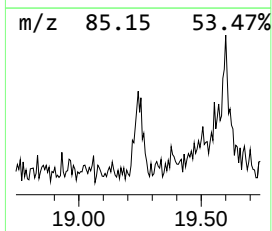
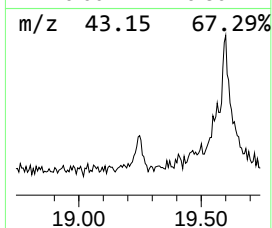
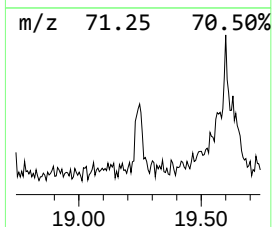
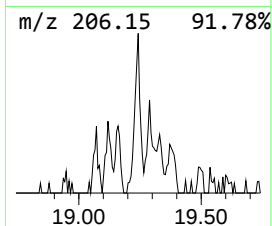
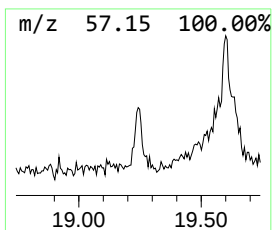
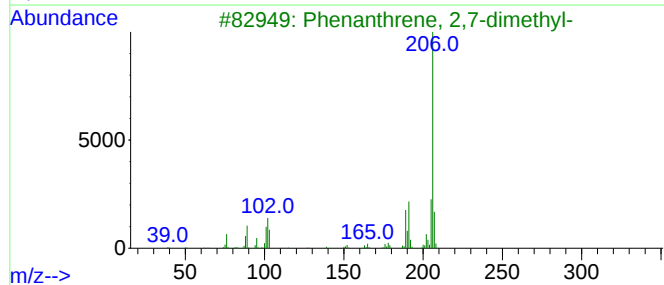
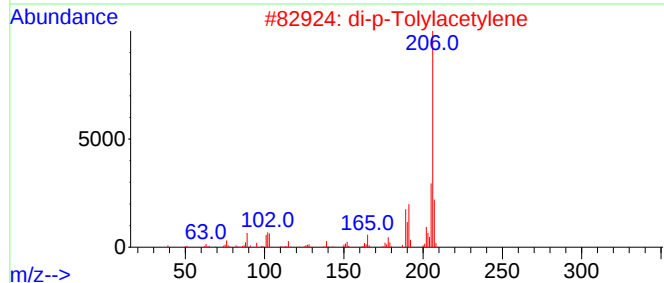
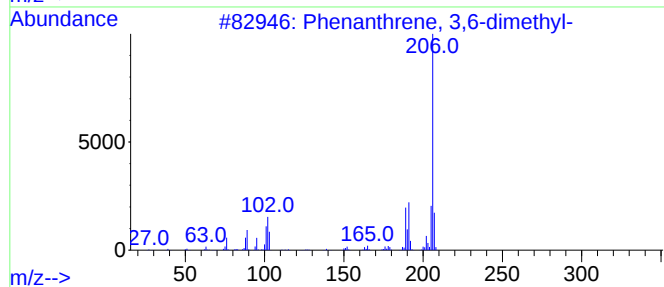
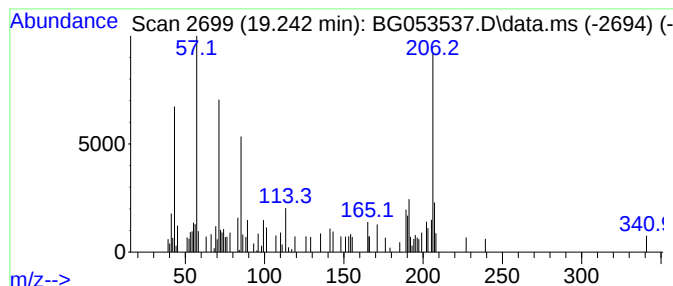
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Phenanthrene, 3,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.242	3.21 ng	62376	Phenanthrene-d10	17.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	55
2			di-p-Tolylacetylene	206	C16H14	002789-88-0	49
3			Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	49
4			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	49
5			3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	46



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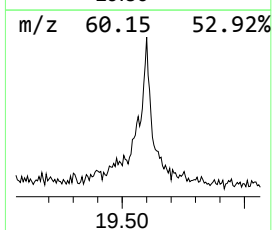
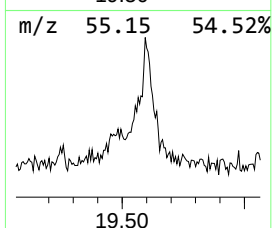
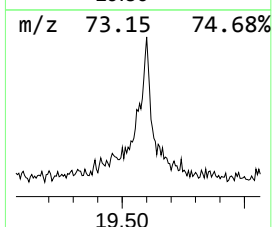
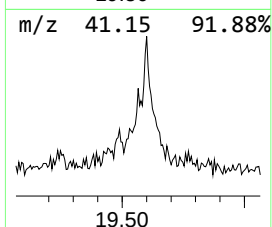
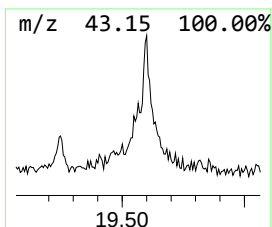
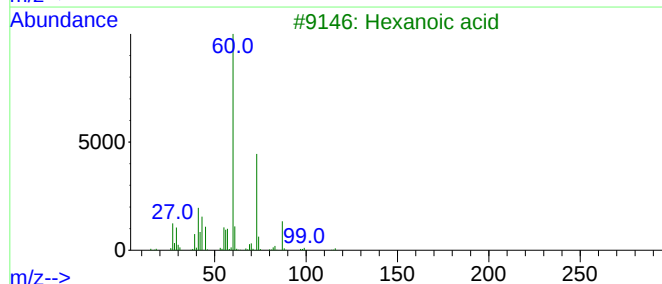
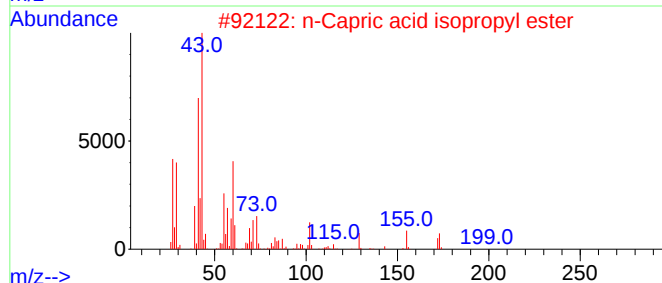
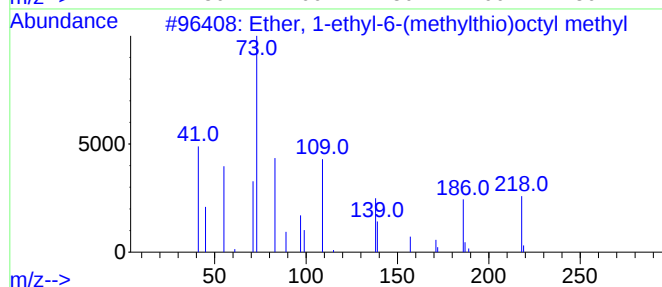
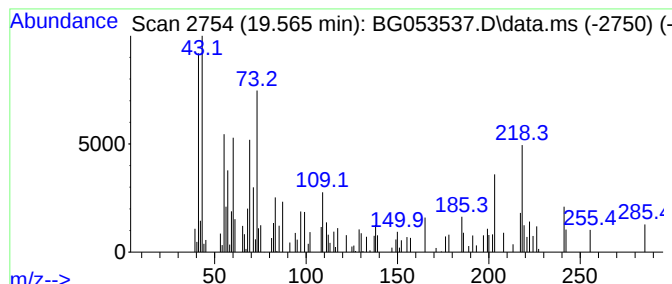
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown19.565 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.565	3.76 ng	72978	Phenanthrene-d10	17.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ether, 1-ethyl-6-(methylthio)oct...	218	C12H26OS	030571-77-8	22
2			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	14
3			Hexanoic acid	116	C6H12O2	000142-62-1	10
4			d-Lyxose	150	C5H10O5	001114-34-7	10
5			Dodecanoic acid	200	C12H24O2	000143-07-7	10



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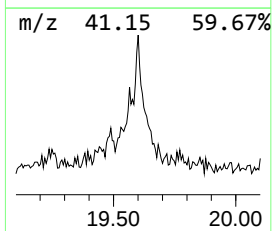
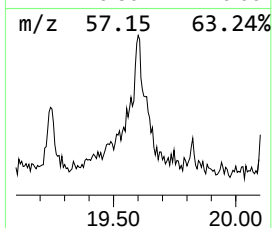
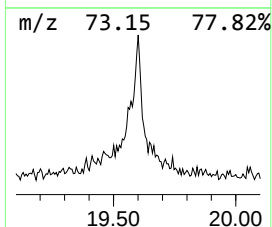
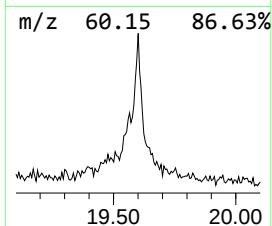
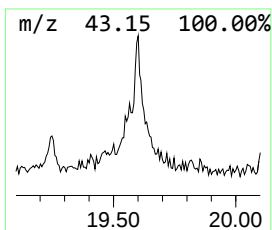
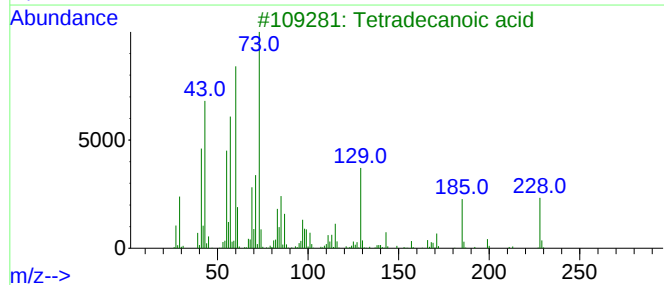
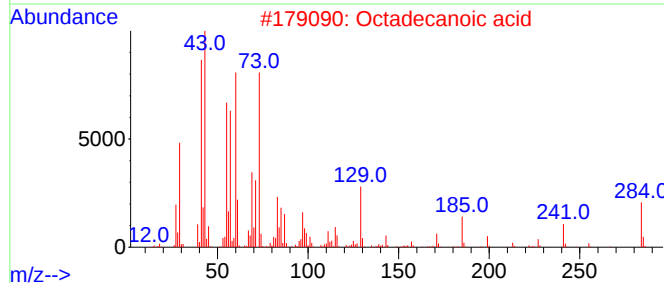
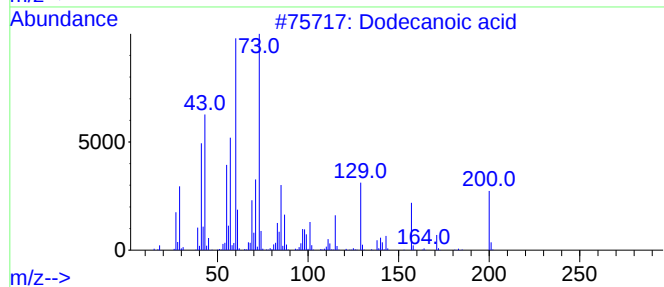
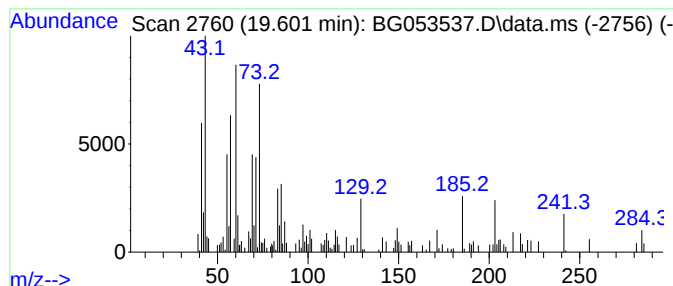
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.601	6.67 ng	227816	Chrysene-d12	21.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	64
2			Octadecanoic acid	284	C18H36O2	000057-11-4	62
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			Tridecanoic acid	214	C13H26O2	000638-53-9	49
5			n-Decanoic acid	172	C10H20O2	000334-48-5	49



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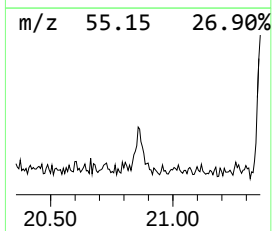
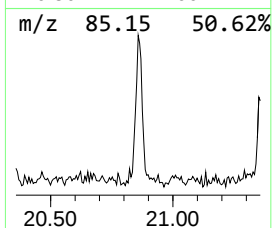
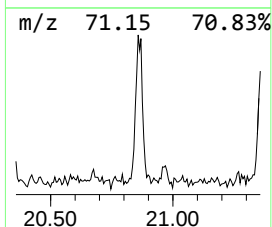
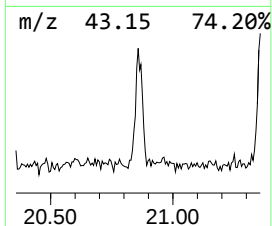
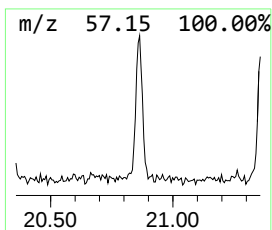
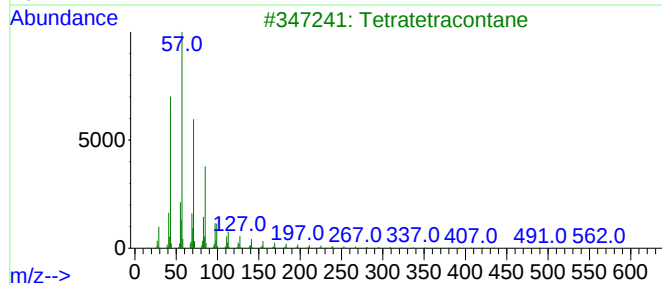
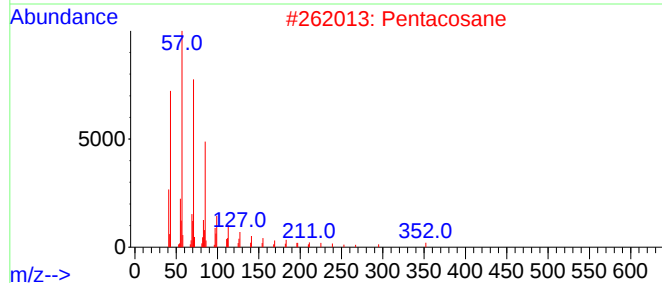
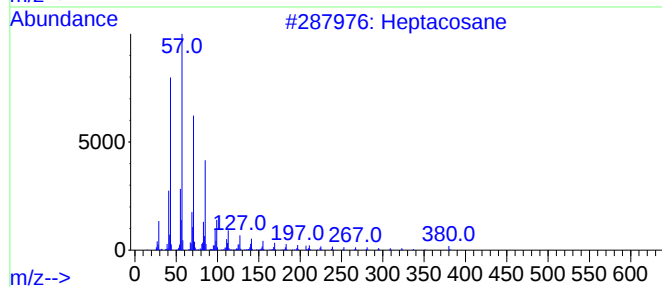
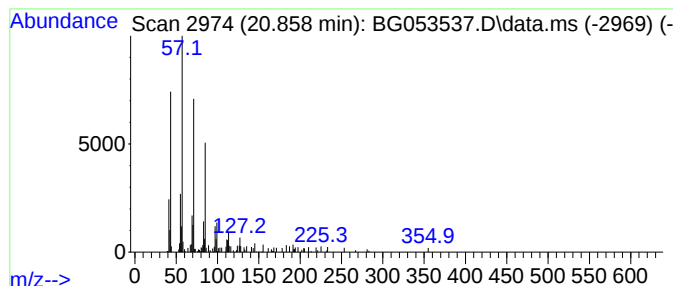
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.858	2.56 ng	87502	Chrysene-d12	21.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Pentacosane	352	C25H52	000629-99-2	91
3			Tetratetracontane	619	C44H90	007098-22-8	90
4			Eicosane	282	C20H42	000112-95-8	87
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053537.D
Acq On : 13 May 2022 11:05
Operator : CG/JU
Sample : N2749-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

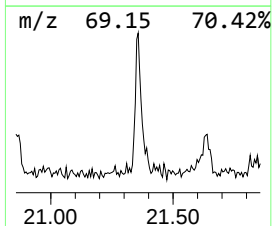
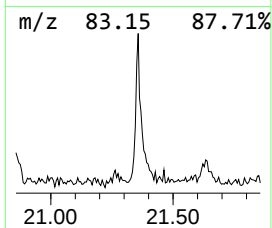
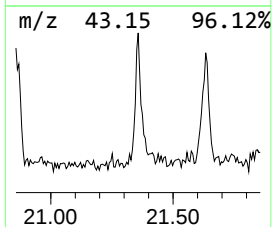
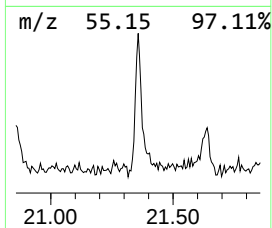
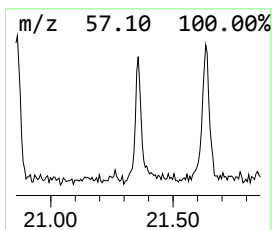
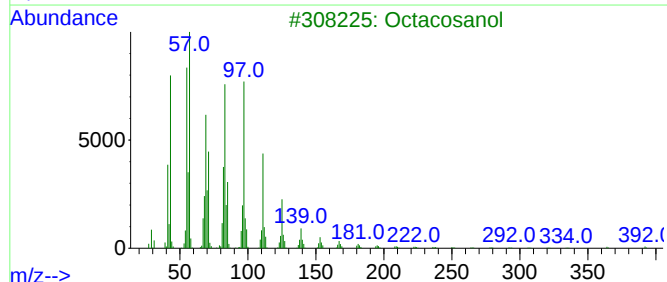
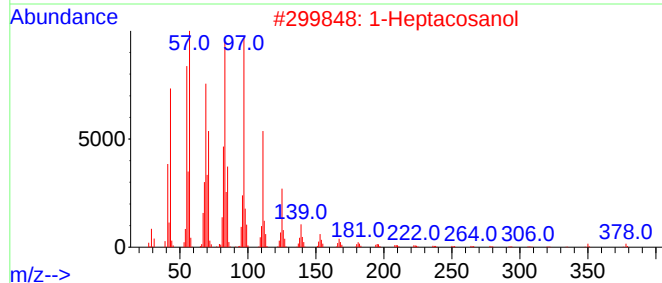
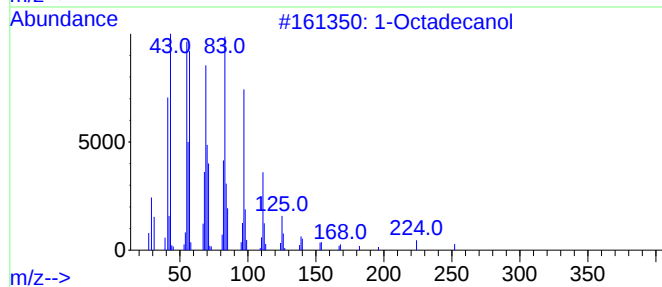
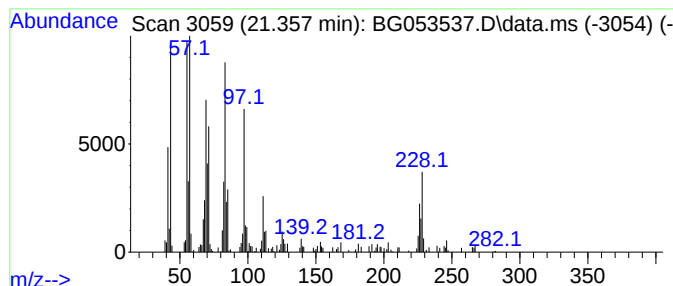
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Octadecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.357	4.01 ng	137020	Chrysene-d12	21.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol			270	C18H38O	000112-92-5	76
2	1-Heptacosanol			396	C27H56O	002004-39-9	68
3	Octacosanol			410	C28H58O	000557-61-9	62
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	62
5	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053537.D
Acq On : 13 May 2022 11:05
Operator : CG/JU
Sample : N2749-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

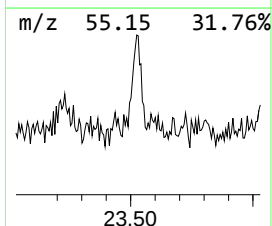
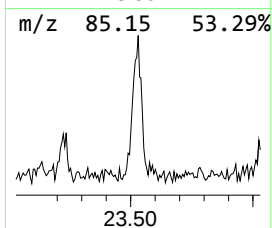
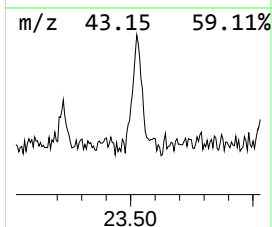
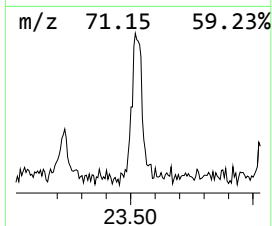
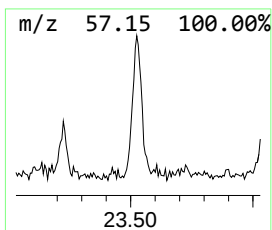
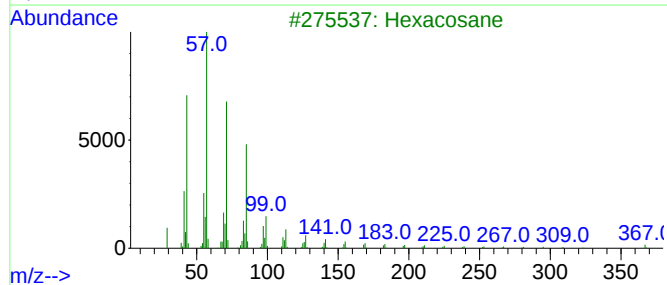
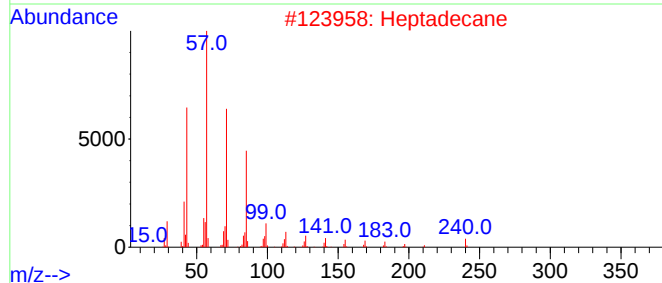
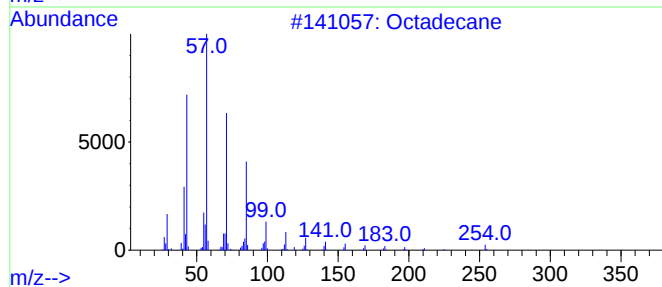
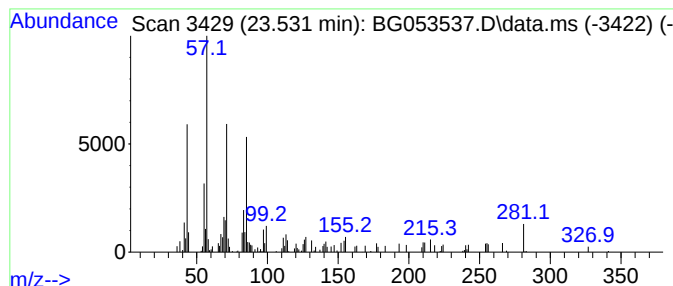
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.531	3.30 ng	91108	Perylene-d12	25.005

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	96
2			Heptadecane	240	C17H36	000629-78-7	89
3			Hexacosane	366	C26H54	000630-01-3	68
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	64
5			Nonadecane	268	C19H40	000629-92-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053537.D
Acq On : 13 May 2022 11:05
Operator : CG/JU
Sample : N2749-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

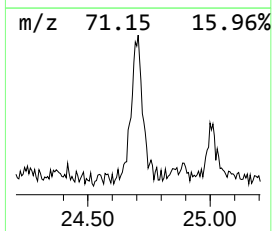
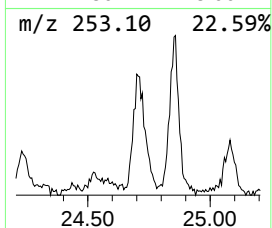
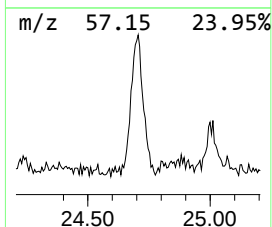
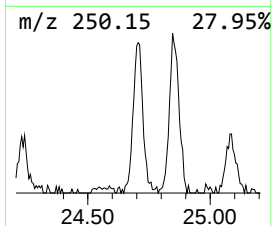
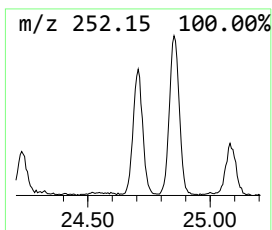
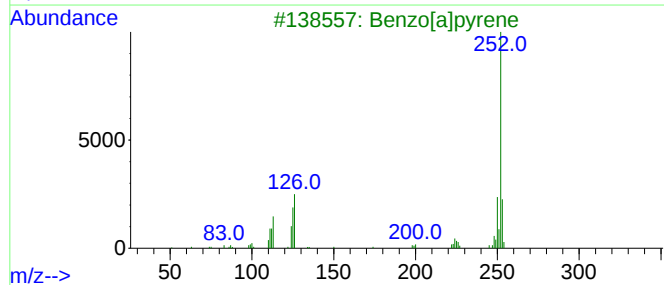
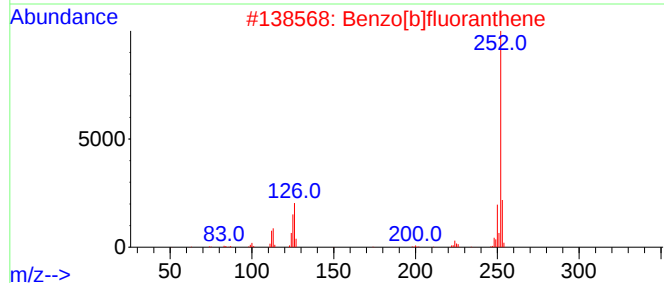
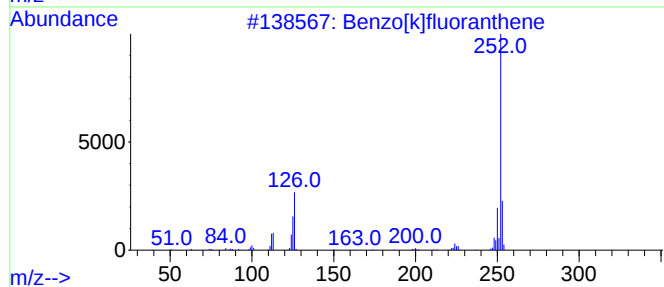
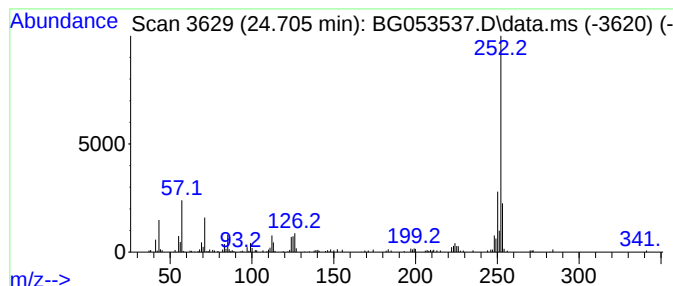
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.705	10.54 ng	291006	Perylene-d12	25.005

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
3			Benzo[a]pyrene	252	C20H12	000050-32-8	90
4			Perylene	252	C20H12	000198-55-0	81
5			Benzo[e]pyrene	252	C20H12	000192-97-2	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053537.D
Acq On : 13 May 2022 11:05
Operator : CG/JU
Sample : N2749-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

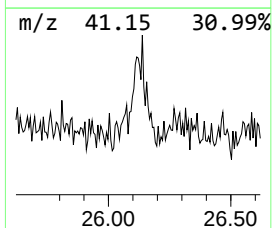
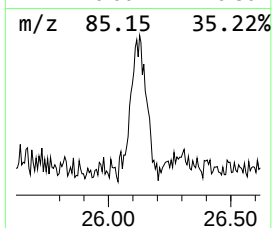
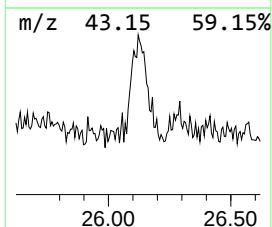
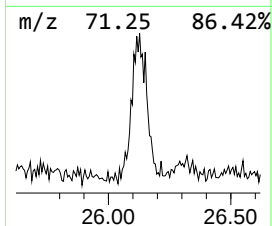
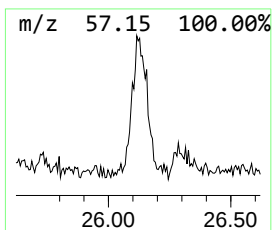
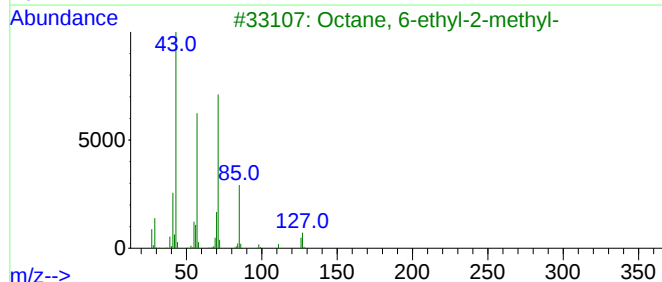
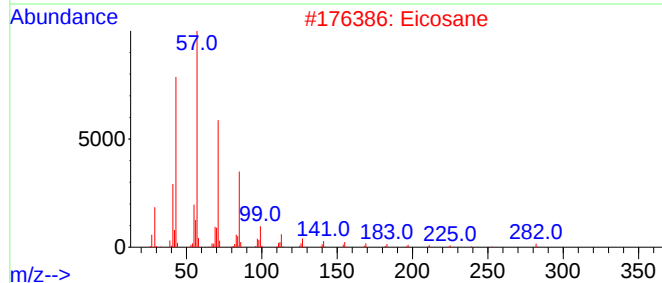
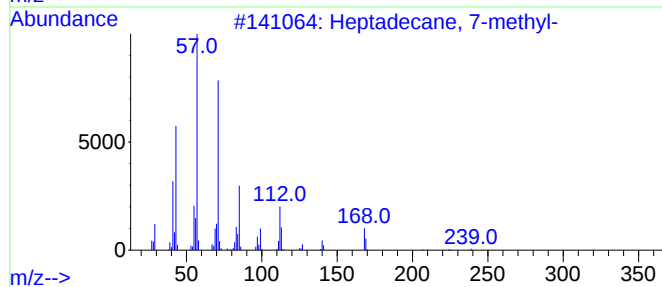
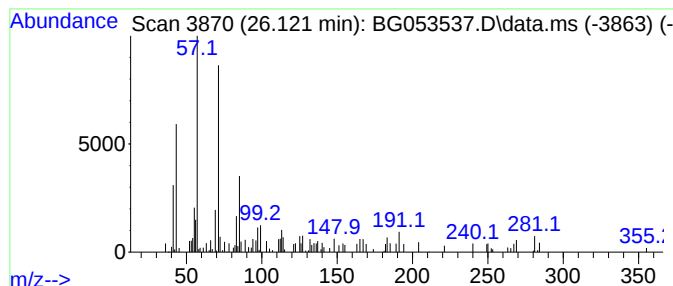
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 7-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.121	3.96 ng	109367	Perylene-d12	25.005

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	50
2			Eicosane	282	C20H42	000112-95-8	50
3			Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	50
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	50
5			Heptadecane	240	C17H36	000629-78-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051322\
Data File : BG053537.D
Acq On : 13 May 2022 11:05
Operator : CG/JU
Sample : N2749-19
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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Phenanthrene, 3...	19.242	3.2	ng	62376	4	17.456	388407	20.0
unknown19.565	19.565	3.8	ng	72978	4	17.456	388407	20.0
Dodecanoic acid	19.601	6.7	ng	227816	5	21.733	682925	20.0
Heptacosane	20.858	2.6	ng	87502	5	21.733	682925	20.0
1-Octadecanol	21.357	4.0	ng	137020	5	21.733	682925	20.0
Octadecane	23.531	3.3	ng	91108	6	25.005	552428	20.0
Perylene	24.705	10.5	ng	291006	6	25.005	552428	20.0
Heptadecane, 7-...	26.121	4.0	ng	109367	6	25.005	552428	20.0