

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
 Data File : BG045484.D
 Acq On : 27 May 2020 20:18
 Operator : CG/JU
 Sample : L2744-19
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NM38-COMP-2020-0-6

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BG051520.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.560	413	421	435	rBV	724910	1267263	36.81%	4.665%
2	7.170	688	695	708	rBV	804925	1481432	43.04%	5.453%
3	7.957	821	829	838	rBV	328538	586258	17.03%	2.158%
4	8.286	877	885	893	rBV	761441	1367192	39.72%	5.032%
5	9.120	1018	1027	1041	rBV	570051	1082516	31.45%	3.985%
6	10.765	1298	1307	1314	rBV	445970	833489	24.21%	3.068%
7	13.221	1718	1725	1736	rBV	1651276	2706947	78.64%	9.964%
8	14.049	1860	1866	1875	rBV	235065	374104	10.87%	1.377%
9	14.601	1952	1960	1967	rBV	736555	1178102	34.22%	4.336%
10	14.666	1967	1971	1977	rVB3	33745	52219	1.52%	0.192%
11	15.006	2023	2029	2032	rBV2	24016	40777	1.18%	0.150%
12	15.653	2131	2139	2146	rBV3	32221	60122	1.75%	0.221%
13	16.099	2207	2215	2226	rBV	1235534	1977775	57.46%	7.280%
14	16.998	2365	2368	2374	rVB2	22449	36490	1.06%	0.134%
15	17.168	2390	2397	2404	rVB3	25833	50160	1.46%	0.185%
16	17.350	2421	2428	2432	rBV	884491	1366650	39.70%	5.030%
17	17.391	2432	2435	2442	rVV	385980	567092	16.47%	2.087%
18	17.480	2443	2450	2455	rVB	69309	115763	3.36%	0.426%
19	17.756	2492	2497	2502	rBV	30030	51875	1.51%	0.191%
20	18.226	2572	2577	2580	rBV	57904	98728	2.87%	0.363%
21	18.273	2580	2585	2591	rVV	88596	171143	4.97%	0.630%
22	18.355	2594	2599	2605	rBV2	23609	47186	1.37%	0.174%
23	18.419	2605	2610	2614	rVV3	74317	149074	4.33%	0.549%
24	18.455	2614	2616	2621	rVB2	41343	56438	1.64%	0.208%
25	18.725	2658	2662	2665	rVV	37610	54140	1.57%	0.199%
26	18.766	2665	2669	2674	rVB5	33094	54975	1.60%	0.202%
27	19.136	2728	2732	2738	rBV	40106	75479	2.19%	0.278%
28	19.277	2752	2756	2760	rBV2	34728	60557	1.76%	0.223%
29	19.400	2771	2777	2783	rVB	497852	719921	20.91%	2.650%
30	19.647	2815	2819	2822	rBV	21734	36396	1.06%	0.134%
31	19.759	2829	2838	2847	rBV	417561	786080	22.84%	2.893%
32	19.841	2848	2852	2856	rVB4	29681	50765	1.47%	0.187%
33	19.964	2866	2873	2879	rBV	2596675	3442296	100.00%	12.670%
34	20.088	2889	2894	2895	rBV3	37659	54498	1.58%	0.201%

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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 >
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35	20.252	2919	2922	2931	rVB2	59457	99443	2.89%	0.366%
36	20.411	2947	2949	2953	rVB2	46759	52945	1.54%	0.195%
37	21.016	3048	3052	3058	rVB	50970	81720	2.37%	0.301%
38	21.269	3091	3095	3103	rVB5	141506	266900	7.75%	0.982%
39	21.498	3132	3134	3140	rVB	39433	55882	1.62%	0.206%
40	21.603	3145	3152	3158	rVV3	843036	1740993	50.58%	6.408%
41	21.656	3158	3161	3173	rVB	183021	303222	8.81%	1.116%
42	21.803	3183	3186	3193	rVB3	62232	104142	3.03%	0.383%
43	22.408	3285	3289	3294	rVB3	79346	127635	3.71%	0.470%
44	23.084	3400	3404	3411	rVB3	89596	165777	4.82%	0.610%
45	23.272	3431	3436	3442	rVB	155507	307394	8.93%	1.131%
46	23.759	3513	3519	3527	rBV	112624	347268	10.09%	1.278%
47	23.871	3535	3538	3545	rVB2	95367	175446	5.10%	0.646%
48	24.458	3635	3638	3649	rVB	72201	177949	5.17%	0.655%
49	24.605	3657	3663	3673	rVB	98563	257393	7.48%	0.947%
50	24.758	3679	3689	3706	rBV2	467802	1613569	46.87%	5.939%
51	25.898	3879	3883	3893	rVB3	84781	236256	6.86%	0.870%

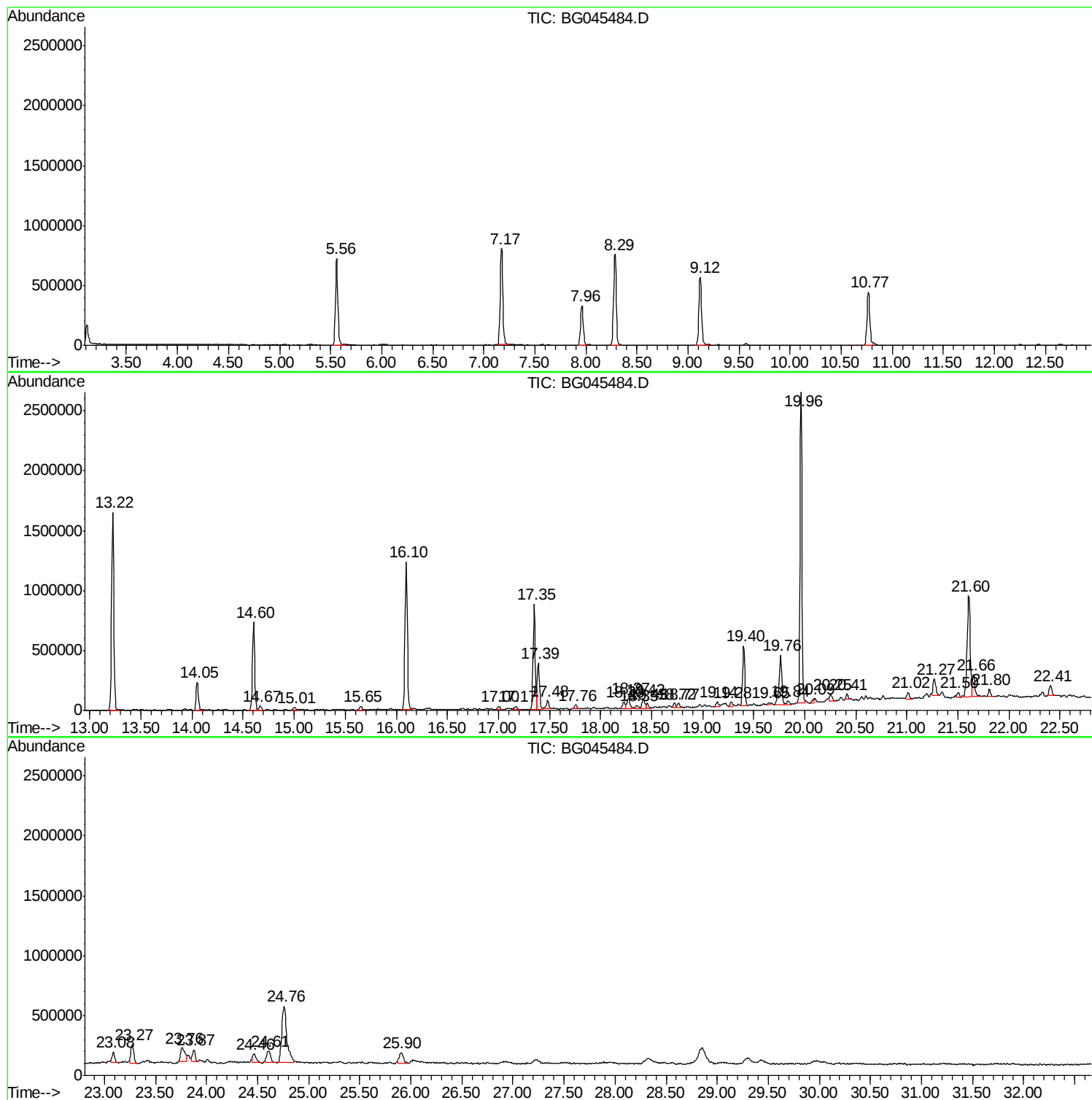
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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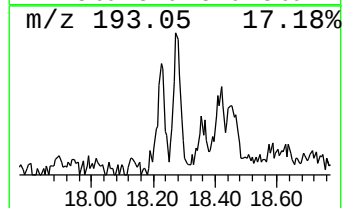
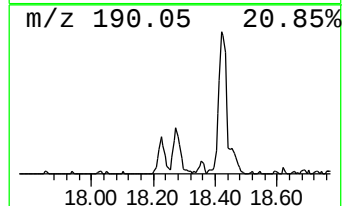
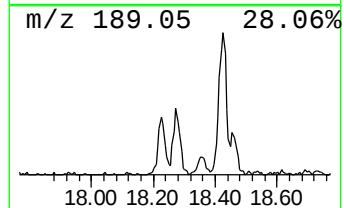
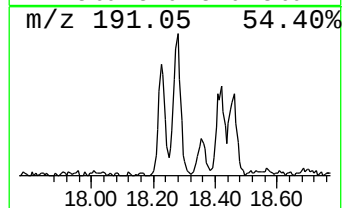
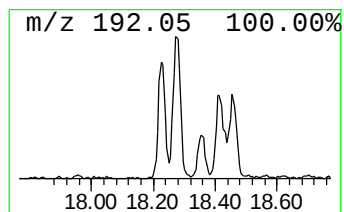
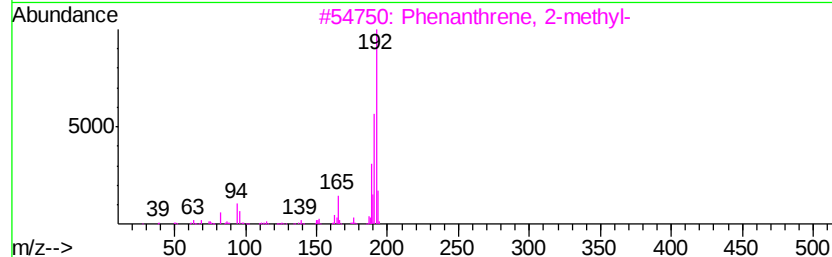
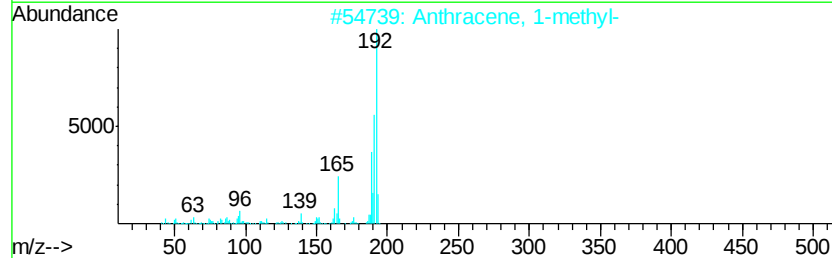
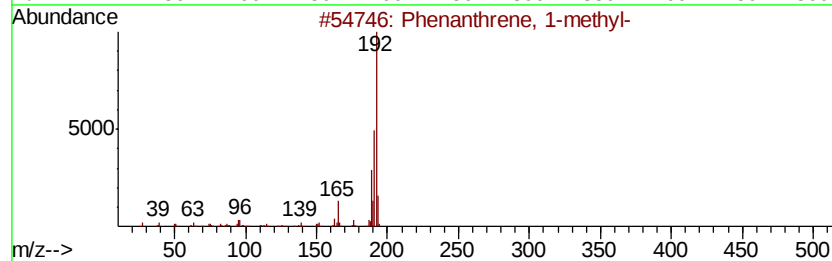
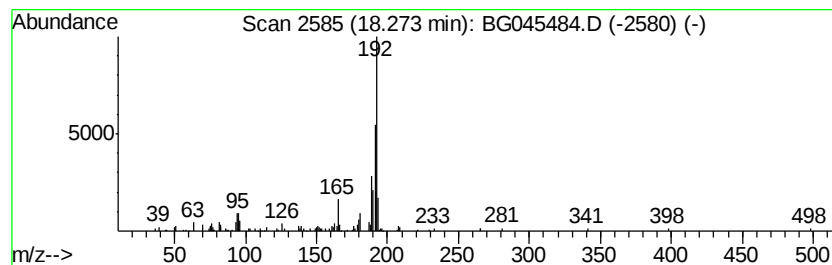
Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.27	2.50 ng	171143	Phenanthrene-d10	17.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
4	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	89
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87



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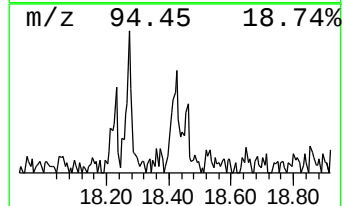
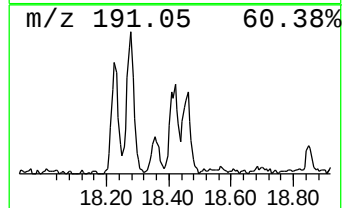
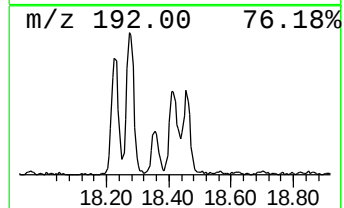
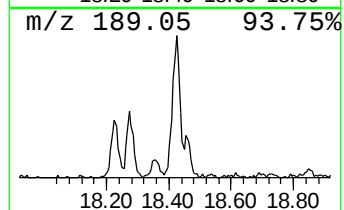
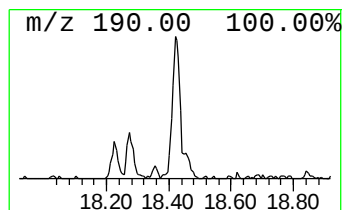
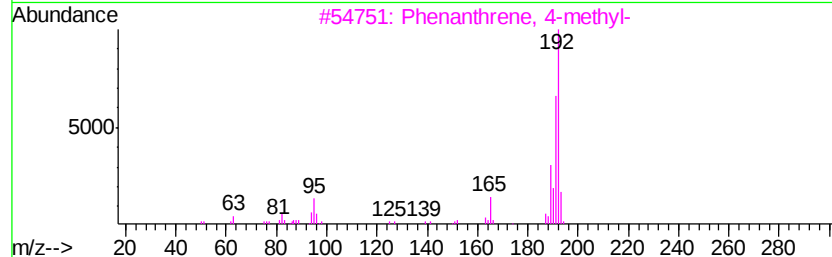
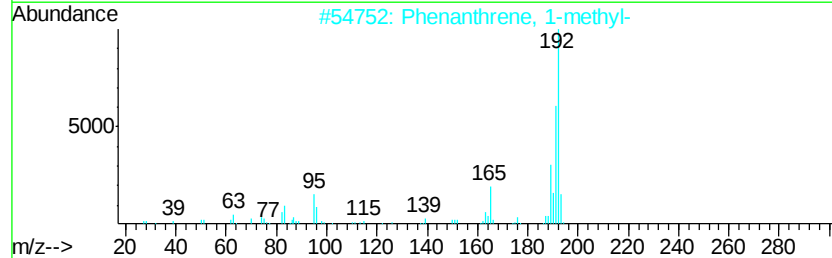
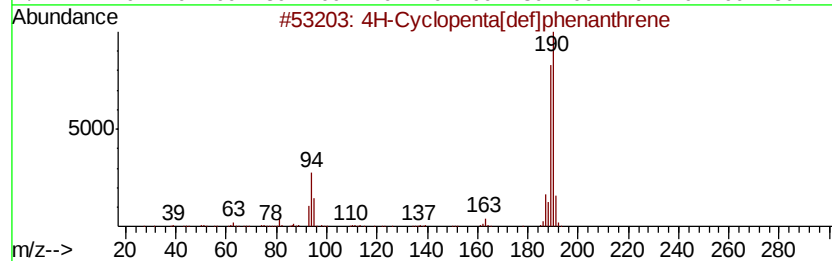
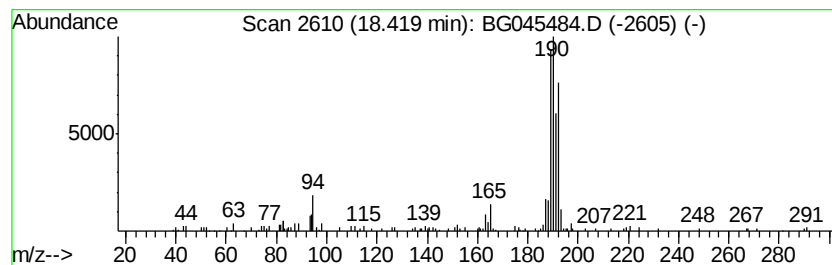
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.42	2.18 ng	149074	Phenanthrene-d10	17.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	42
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
4	Methyl diselenide	190	C2H6Se2	007101-31-7	42
5	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	42



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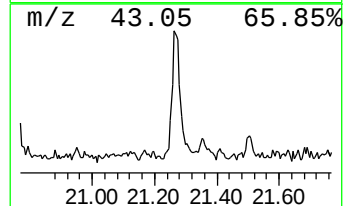
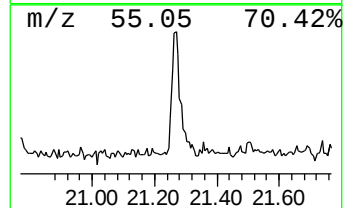
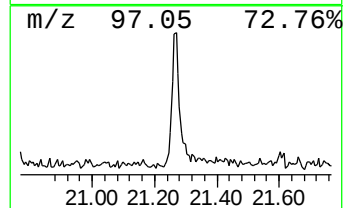
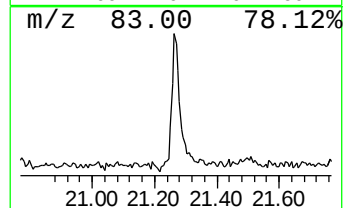
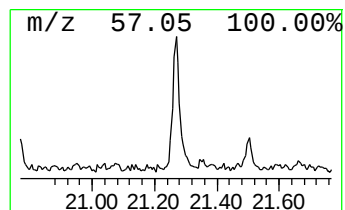
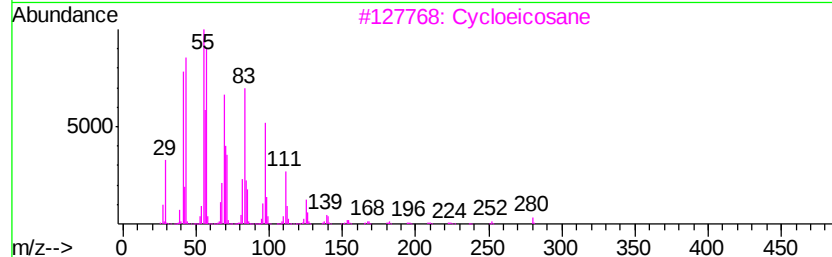
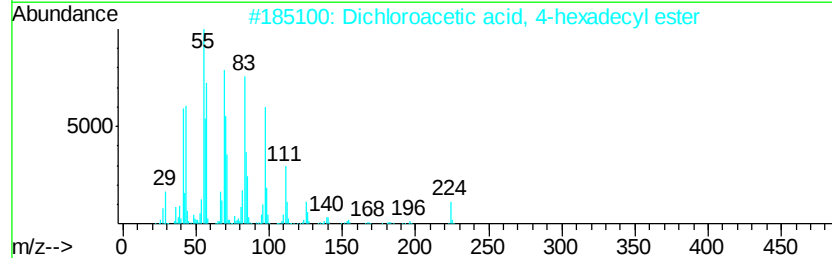
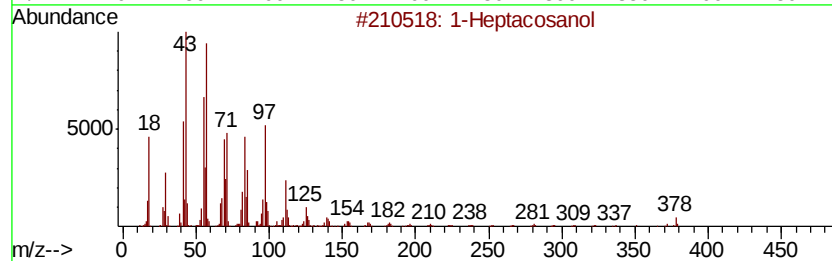
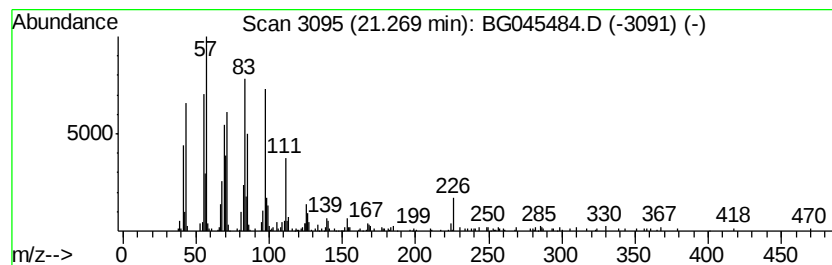
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	3.07 ng	266900	Chrysene-d12	21.61
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol	396 C27H56O	002004-39-9	87
2	Dichloroacetic acid, 4-hexadecyl...	352 C18H34Cl2O2	1000282-98-1	72
3	Cycloeicosane	280 C20H40	000296-56-0	68
4	1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6	62
5	Octacosyl trifluoroacetate	506 C30H57F3O2	1000351-74-9	62



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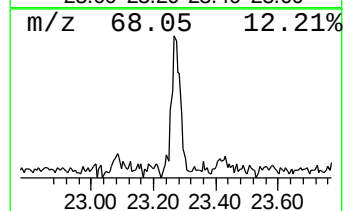
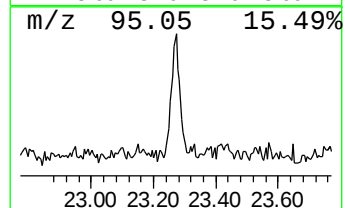
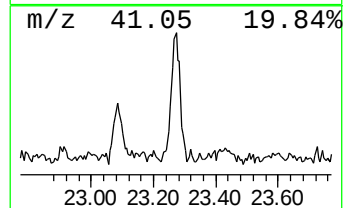
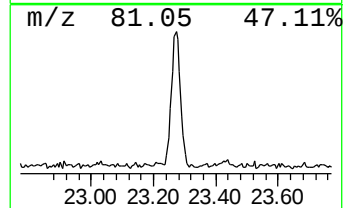
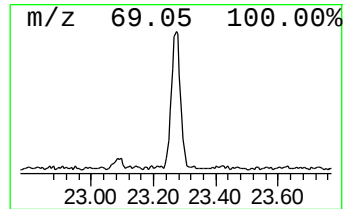
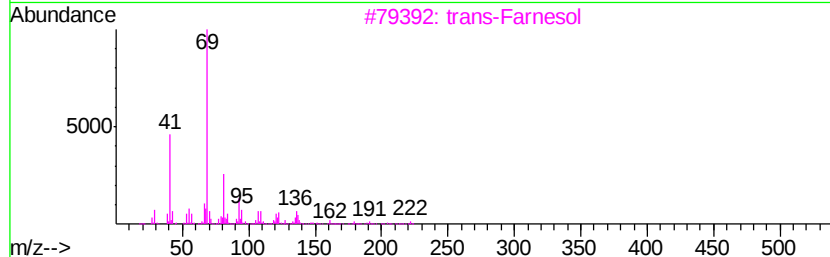
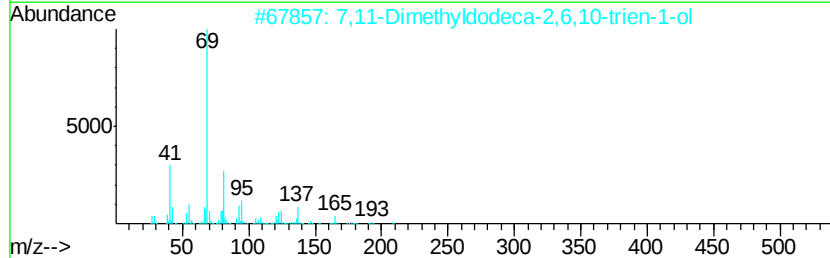
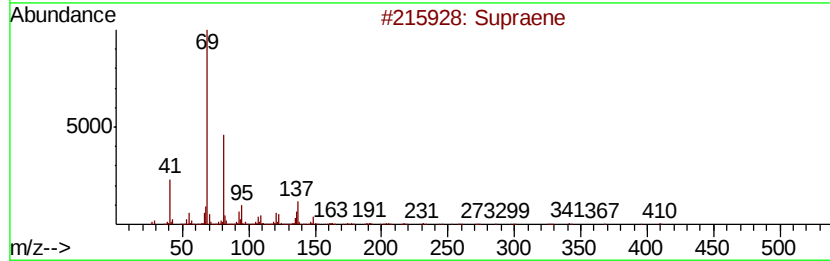
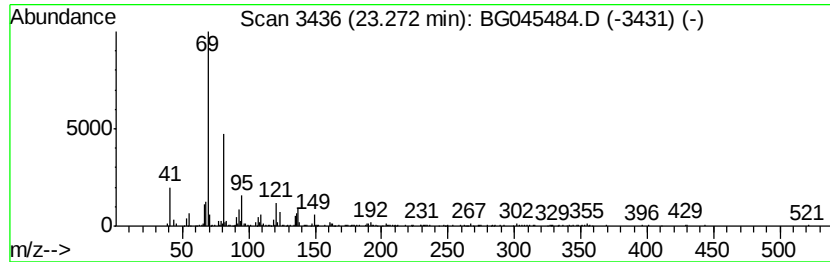
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
23.27	3.81 ng	307394	Perylene-d12		24.76
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	74
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3	trans-Farnesol	222	C15H26O	000106-28-5	72
4	Squalene	410	C30H50	000111-02-4	72
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64



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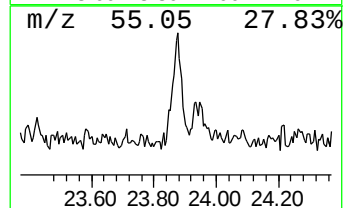
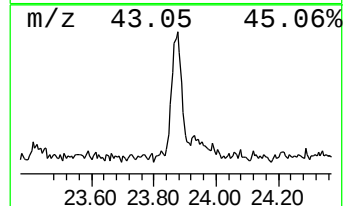
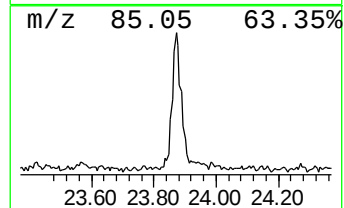
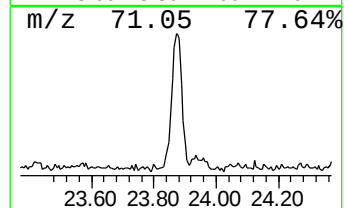
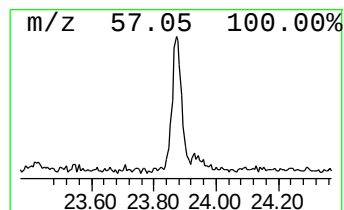
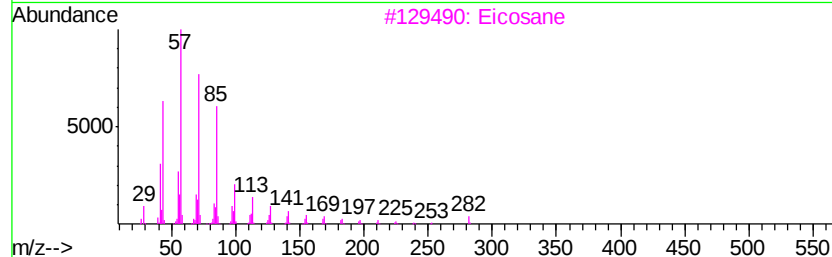
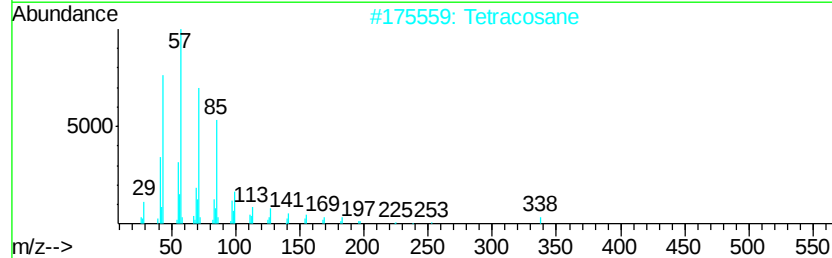
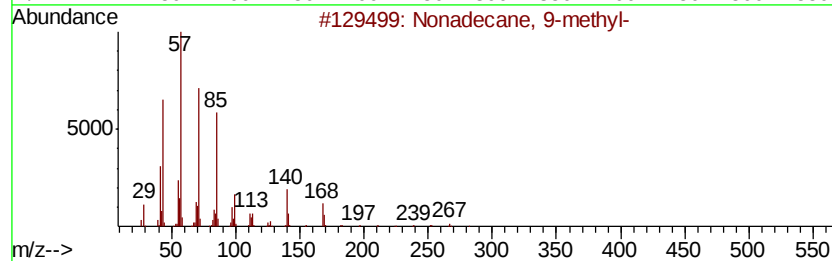
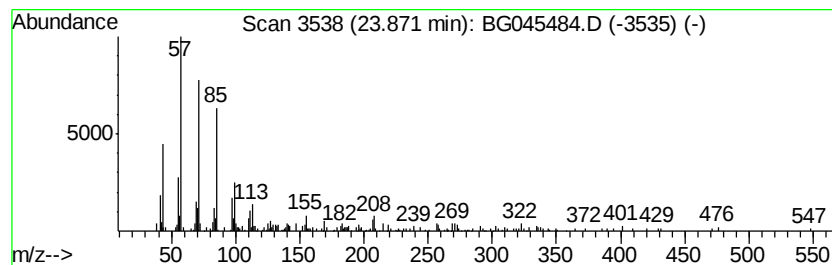
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	2.17 ng	175446	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	90
2		Tetracosane	338	C24H50	000646-31-1	87
3		Eicosane	282	C20H42	000112-95-8	83
4		Dodecane, 2-methyl-	184	C13H28	001560-97-0	81
5		Pentacosane	352	C25H52	000629-99-2	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045484.D
Acq On : 27 May 2020 20:18
Operator : CG/JU
Sample : L2744-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM38-COMP-2020-0-6

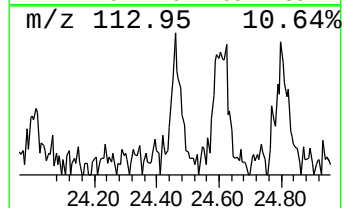
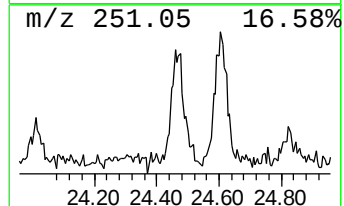
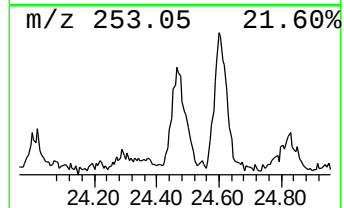
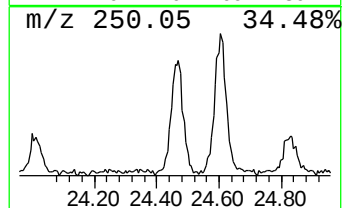
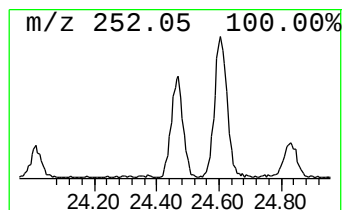
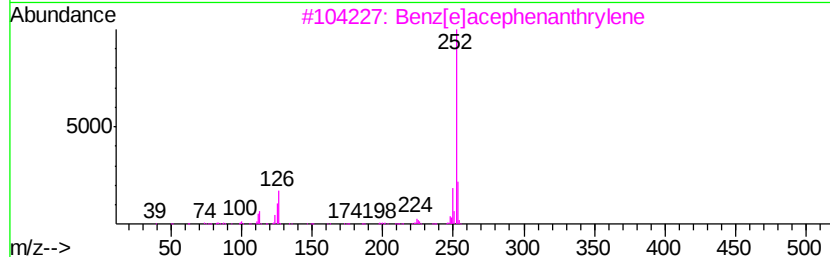
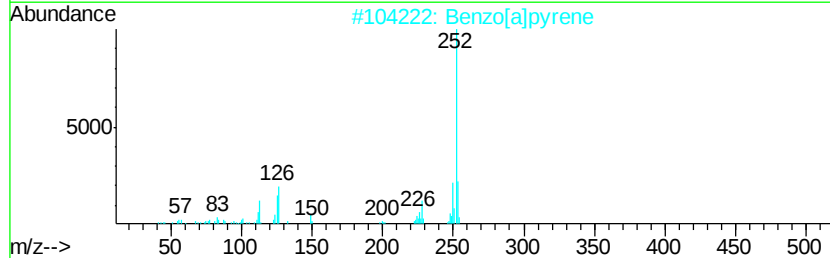
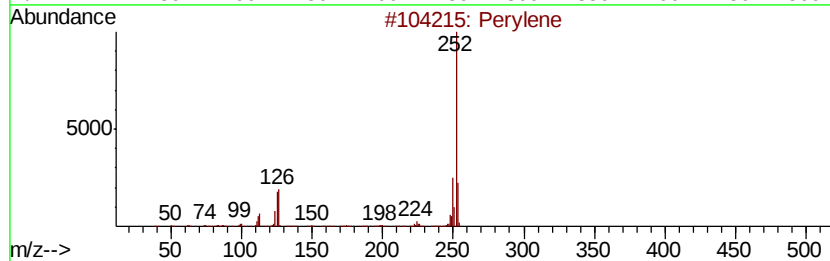
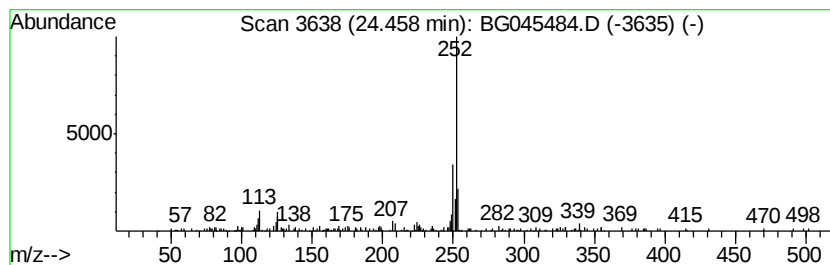
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.46	2.21 ng	177949	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	93
2		Benzo[a]pyrene	252	C20H12	000050-32-8	76
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	70
4		1-Amino-4-(phenylthio)isoquinoline	252	C15H12N2S	019653-19-1	68
5		Benzo[e]pyrene	252	C20H12	000192-97-2	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045484.D
Acq On : 27 May 2020 20:18
Operator : CG/JU
Sample : L2744-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM38-COMP-2020-0-6

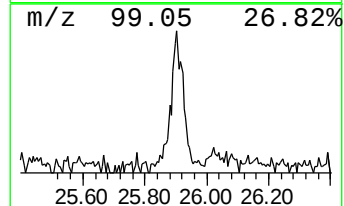
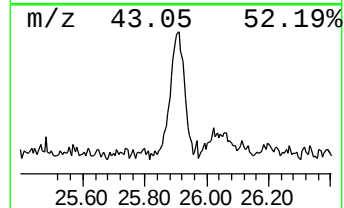
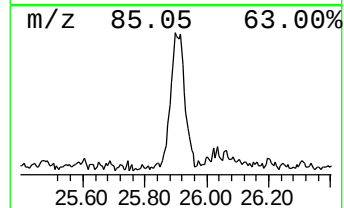
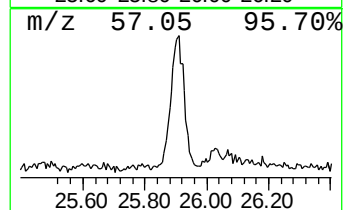
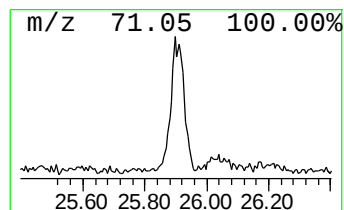
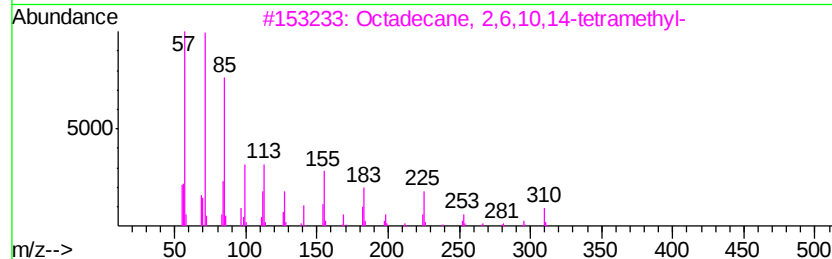
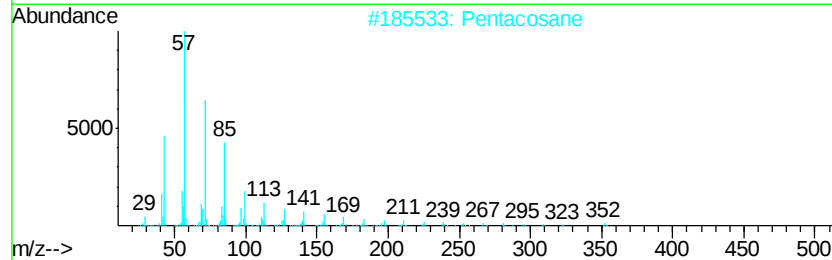
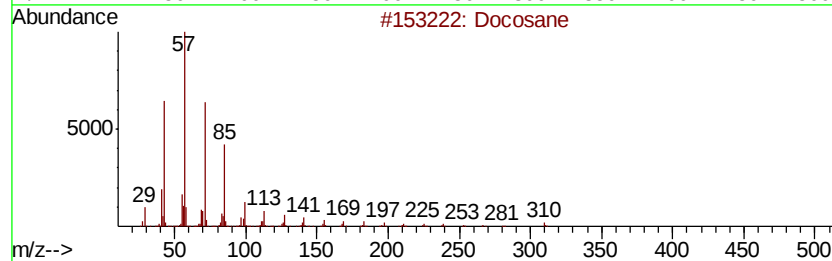
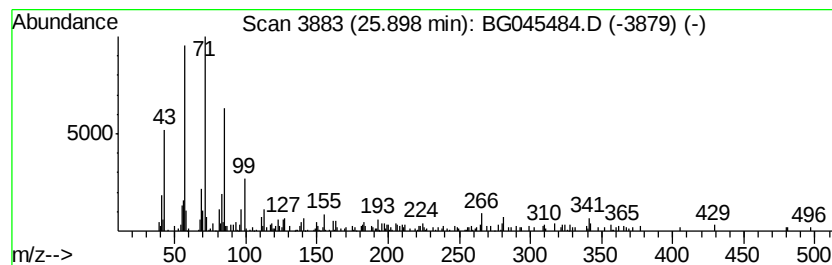
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.90	2.93 ng	236256	Perylene-d12	24.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane		310	C22H46	000629-97-0	89
2	Pentacosane		352	C25H52	000629-99-2	87
3	Octadecane, 2,6,10,14-tetramethyl-		310	C22H46	054964-82-8	80
4	Tridecane, 6-propyl-		226	C16H34	055045-10-8	76
5	Pentadecane		212	C15H32	000629-62-9	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052720\
Data File : BG045484.D
Acq On : 27 May 2020 20:18
Operator : CG/JU
Sample : L2744-19
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM38-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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
Phenanthrene, 1-m...	18.27	2.5	ng	171143	4	17.35	1366650	20.0
4H-Cyclopenta[def...	18.42	2.2	ng	149074	4	17.35	1366650	20.0
1-Heptacosanol	21.27	3.1	ng	266900	5	21.61	1740990	20.0
Supraene	23.27	3.8	ng	307394	6	24.76	1613570	20.0
Nonadecane, 9-met...	23.87	2.2	ng	175446	6	24.76	1613570	20.0
Perylene	24.46	2.2	ng	177949	6	24.76	1613570	20.0
Docosane	25.90	2.9	ng	236256	6	24.76	1613570	20.0