

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
 Data File : BG045486.D
 Acq On : 27 May 2020 21:40
 Operator : CG/JU
 Sample : L2746-13
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NM70-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	5.561	413	421	434	rBV	789054	1388690	35.90%	3.984%
2	7.176	686	696	707	rBV	926038	1697954	43.90%	4.871%
3	7.957	822	829	838	rBV	352804	627502	16.22%	1.800%
4	8.286	876	885	896	rBV	827013	1486962	38.44%	4.266%
5	9.121	1017	1027	1037	rBV	641813	1198500	30.99%	3.438%
6	10.765	1298	1307	1314	rBV	491768	910737	23.55%	2.613%
7	13.227	1718	1726	1735	rBV	1866378	3065646	79.26%	8.794%
8	14.049	1859	1866	1872	rBV	183671	274907	7.11%	0.789%
9	14.601	1952	1960	1967	rBV	803363	1313482	33.96%	3.768%
10	14.666	1967	1971	1977	rVB	41620	66124	1.71%	0.190%
11	15.007	2022	2029	2035	rBV3	24081	41577	1.07%	0.119%
12	15.653	2133	2139	2143	rBV3	40118	65185	1.69%	0.187%
13	16.099	2207	2215	2224	rBV	1476896	2337191	60.43%	6.705%
14	17.004	2363	2369	2375	rVB3	24569	41870	1.08%	0.120%
15	17.351	2421	2428	2432	rBV	945573	1514566	39.16%	4.345%
16	17.392	2432	2435	2441	rVB	462305	667194	17.25%	1.914%
17	17.480	2446	2450	2456	rVB	102112	158309	4.09%	0.454%
18	17.756	2494	2497	2506	rVB	30939	47215	1.22%	0.135%
19	18.226	2573	2577	2580	rBV	73831	109282	2.83%	0.313%
20	18.273	2580	2585	2594	rVB3	115673	246280	6.37%	0.706%
21	18.355	2594	2599	2604	rVB2	42431	63445	1.64%	0.182%
22	18.420	2604	2610	2614	rBV2	123229	244113	6.31%	0.700%
23	18.455	2614	2616	2622	rVB2	55818	75894	1.96%	0.218%
24	18.719	2658	2661	2665	rBV	49857	70063	1.81%	0.201%
25	18.766	2665	2669	2674	rVB3	38795	57080	1.48%	0.164%
26	19.142	2728	2733	2739	rBV2	54496	109133	2.82%	0.313%
27	19.277	2752	2756	2764	rVV4	51599	103146	2.67%	0.296%
28	19.348	2764	2768	2772	rVV	81639	109220	2.82%	0.313%
29	19.401	2772	2777	2784	rVB	931223	1337392	34.58%	3.837%
30	19.765	2829	2839	2847	rBV	825039	1450209	37.49%	4.160%
31	19.835	2848	2851	2857	rVB4	48537	80407	2.08%	0.231%
32	19.965	2866	2873	2879	rBV	2811333	3867883	100.00%	11.096%
33	20.082	2890	2893	2895	rBV3	52704	70814	1.83%	0.203%
34	20.258	2919	2923	2928	rVB	151100	245883	6.36%	0.705%

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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

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35	20.358	2936	2940	2943	rBV	80086	109967	2.84%	0.315%
36	20.411	2946	2949	2954	rVB3	77468	113736	2.94%	0.326%
37	20.552	2971	2973	2977	rVB	43183	45321	1.17%	0.130%
38	20.599	2978	2981	2986	rVV	51956	69114	1.79%	0.198%
39	21.010	3048	3051	3059	rVB	81797	132984	3.44%	0.381%
40	21.198	3077	3083	3086	rBV4	62672	111788	2.89%	0.321%
41	21.263	3090	3094	3103	rVB5	280718	522510	13.51%	1.499%
42	21.604	3144	3152	3157	rBV3	945546	2179478	56.35%	6.252%
43	21.651	3157	3160	3169	rVB	358464	620571	16.04%	1.780%
44	21.803	3183	3186	3193	rVB3	72965	113581	2.94%	0.326%
45	22.408	3285	3289	3298	rVB6	84128	204072	5.28%	0.585%
46	23.765	3512	3520	3527	rBV2	284280	933181	24.13%	2.677%
47	24.470	3633	3640	3654	rVB2	170970	516923	13.36%	1.483%
48	24.605	3656	3663	3673	rVB	230765	639396	16.53%	1.834%
49	24.758	3680	3689	3698	rBV2	497766	1494226	38.63%	4.286%
50	25.904	3877	3884	3893	rVB2	217153	632211	16.35%	1.814%
51	28.858	4378	4387	4403	rVB8	290686	1276415	33.00%	3.662%

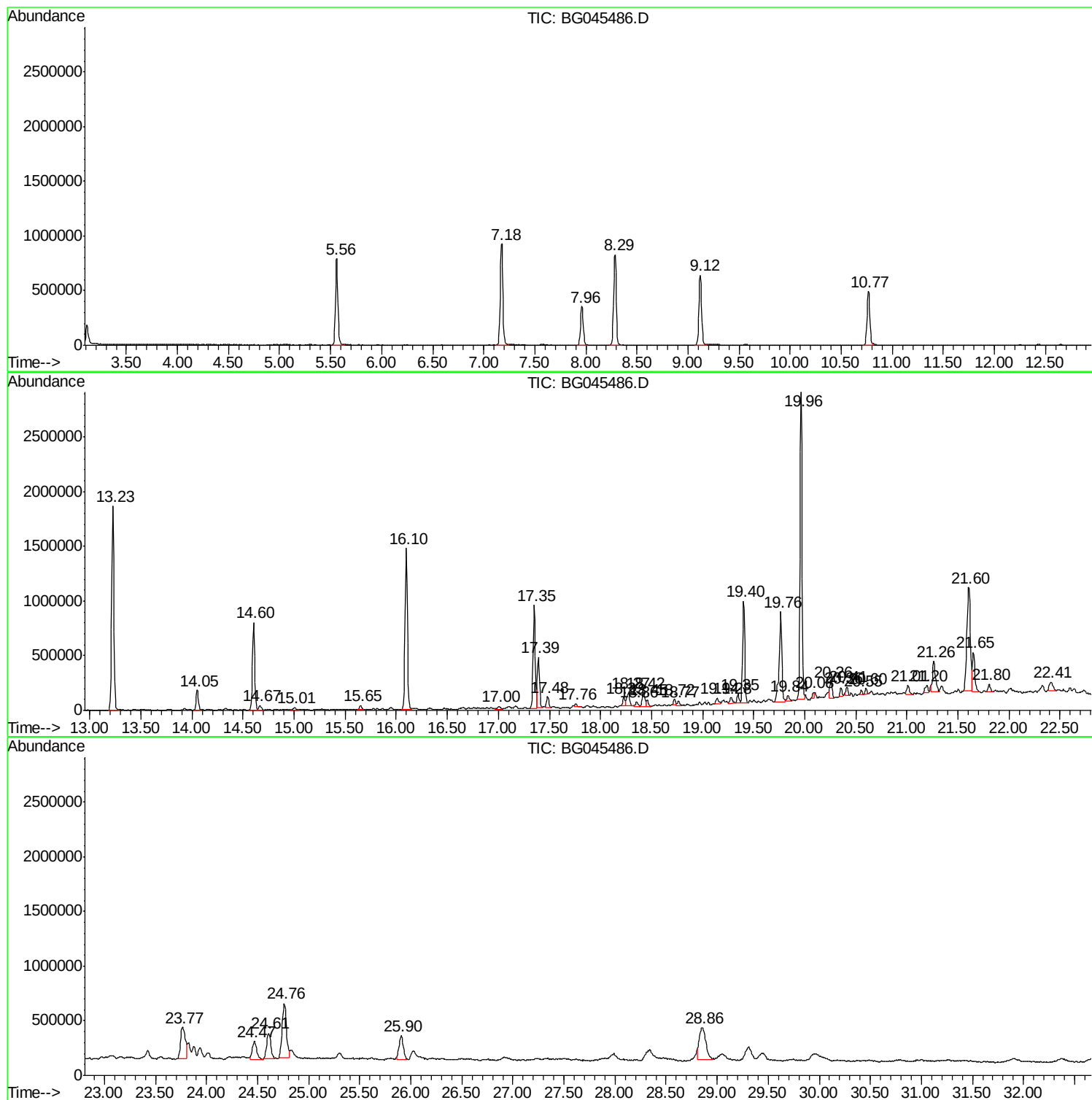
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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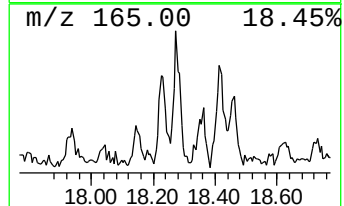
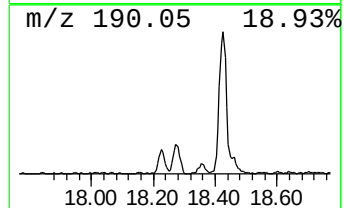
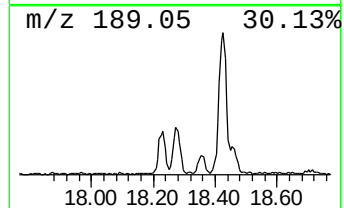
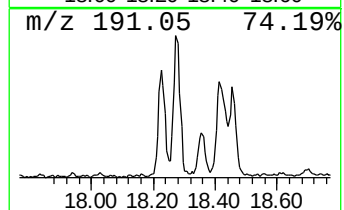
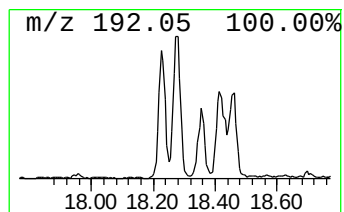
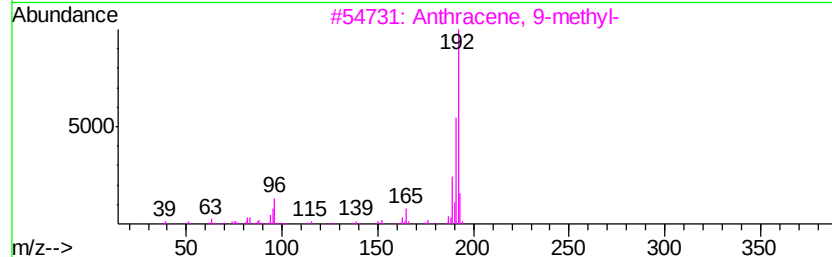
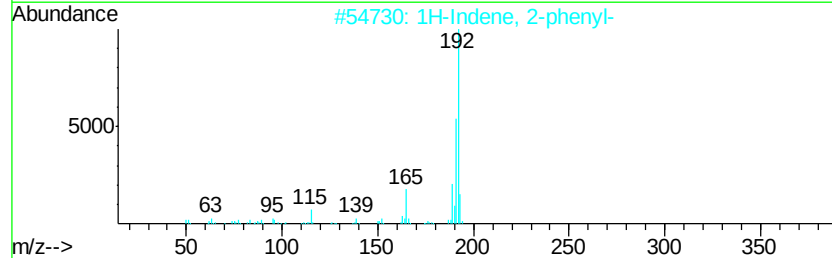
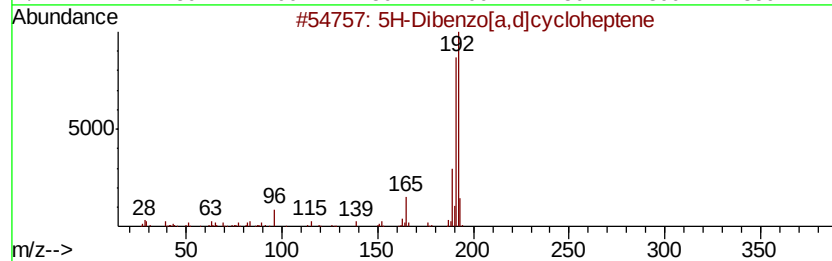
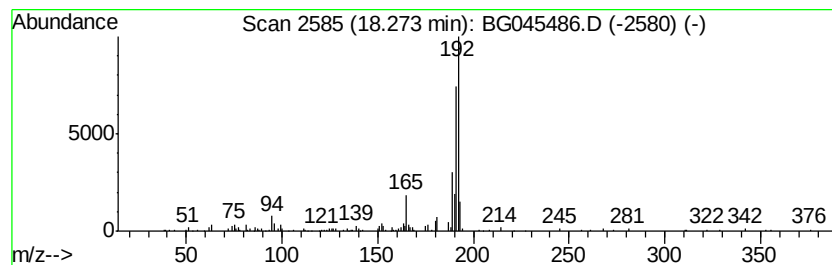
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 5H-Dibenzo[a,d]cycloheptene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.27	3.25 ng	246280	Phenanthrene-d10	17.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	91
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	91
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
4	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	87
5	Benzene, 1,1'-(1,2-propadienyld...	192	C15H12	014251-57-1	87



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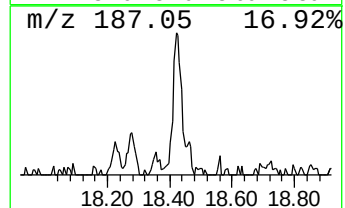
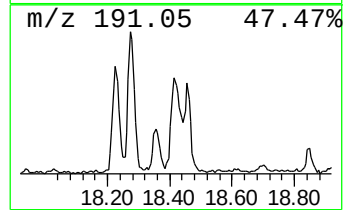
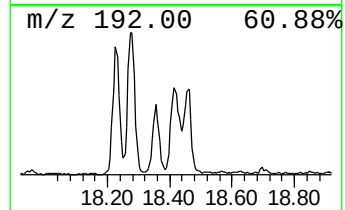
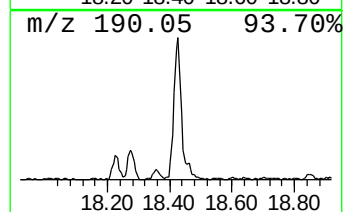
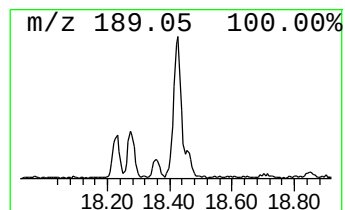
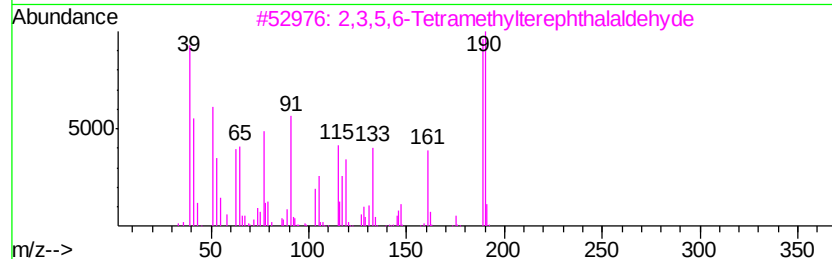
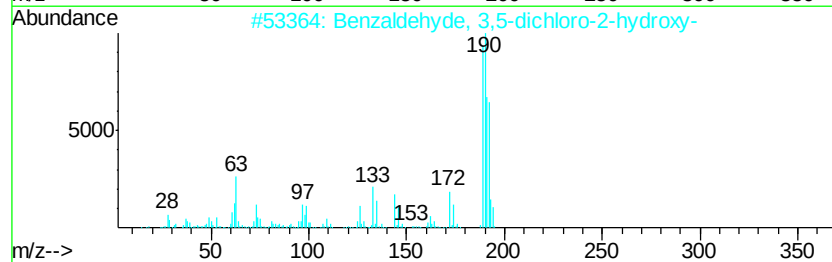
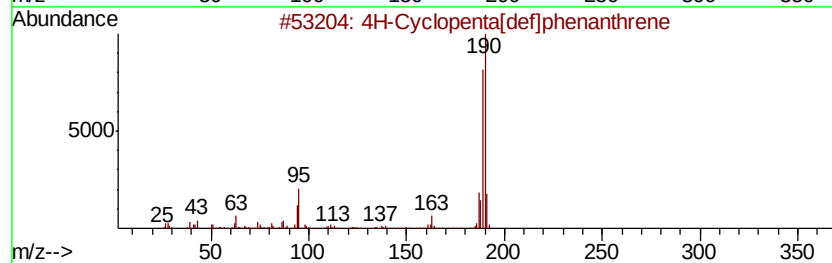
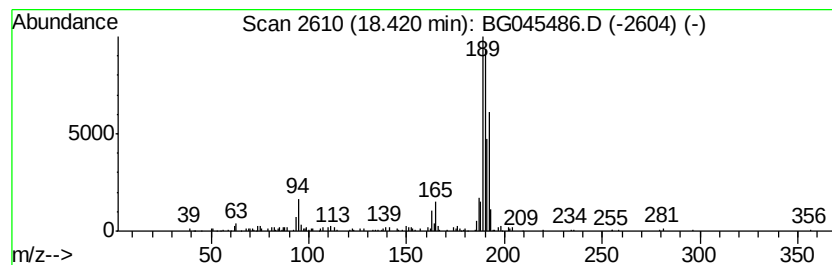
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.42	3.22 ng	244113	Phenanthrene-d10	17.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	64
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	53
3	2,3,5,6-Tetramethylterephthald...	190	C12H14O2	007072-01-7	46
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	38



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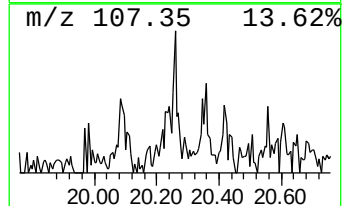
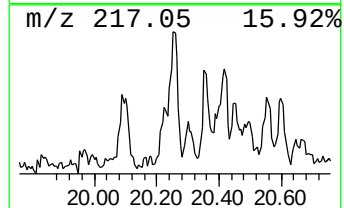
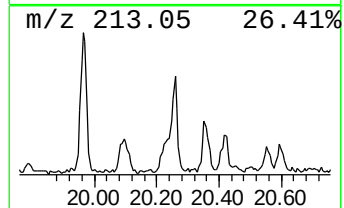
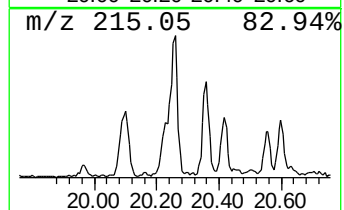
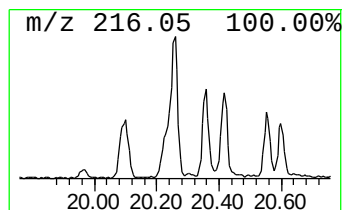
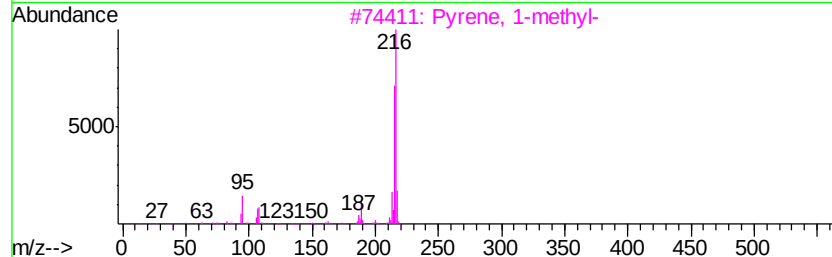
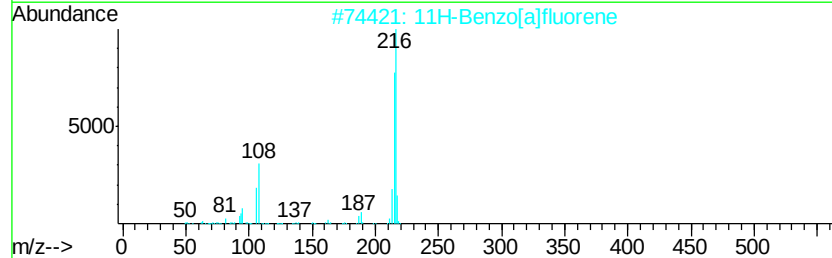
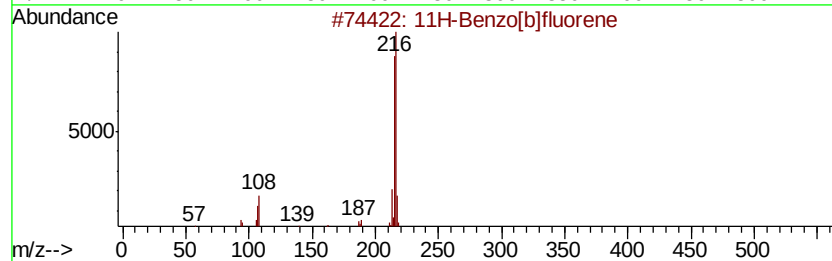
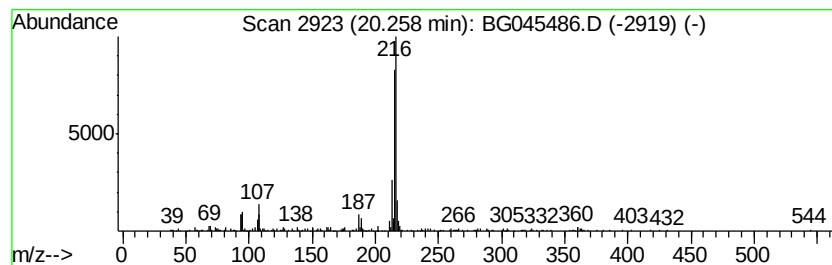
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.26	2.26 ng	245883	Chrysene-d12	21.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3		Pvrene, 1-methyl-	216	C17H12	002381-21-7	83
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72



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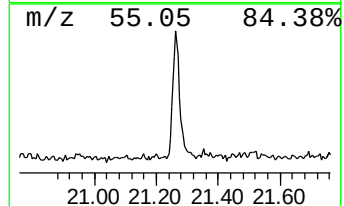
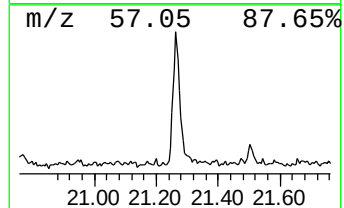
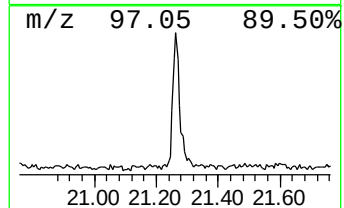
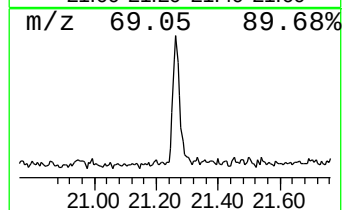
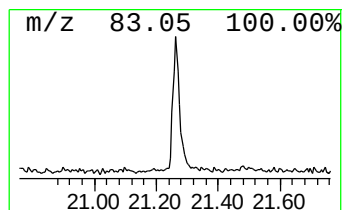
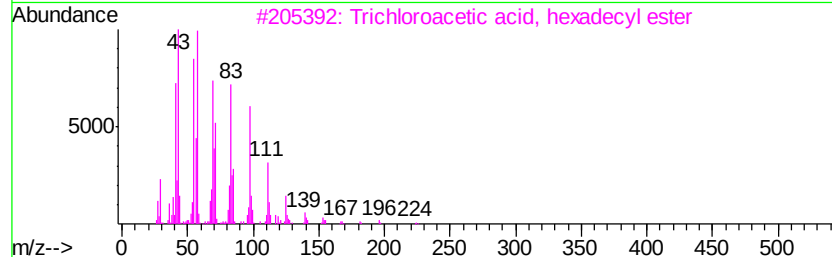
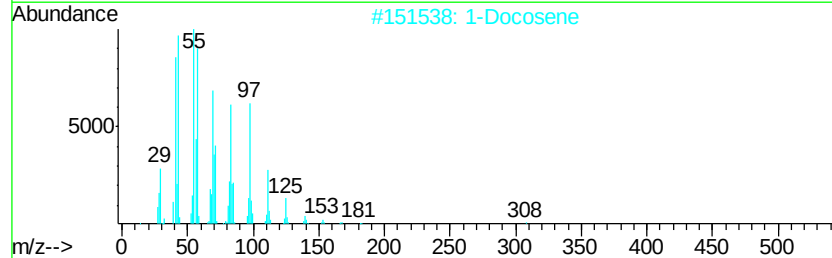
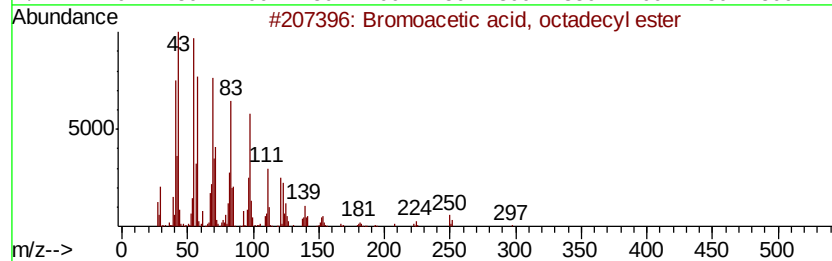
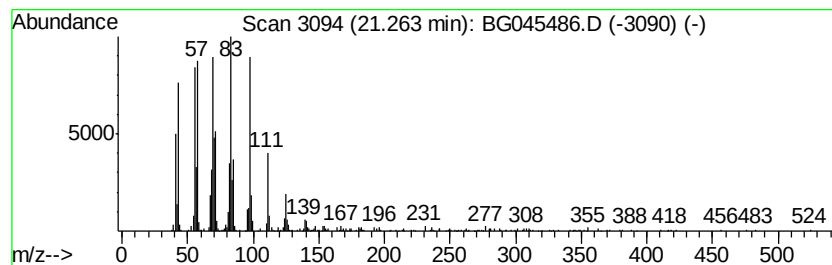
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Bromoacetic acid, octadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.26	4.79 ng	522510	Chrysene-d12	21.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	1-Docosene	308	C22H44	001599-67-3	90
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4	Cyclotetradecane	196	C14H28	000295-17-0	89
5	Cycloeicosane	280	C20H40	000296-56-0	72



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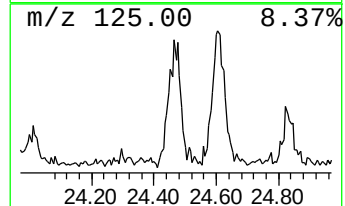
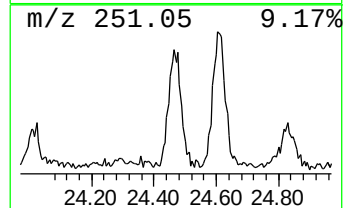
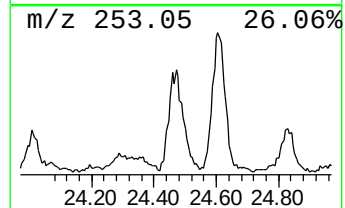
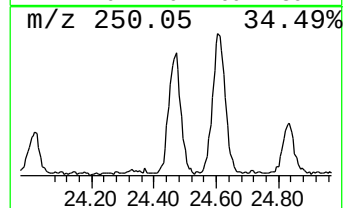
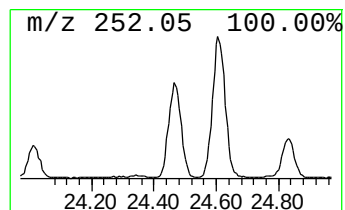
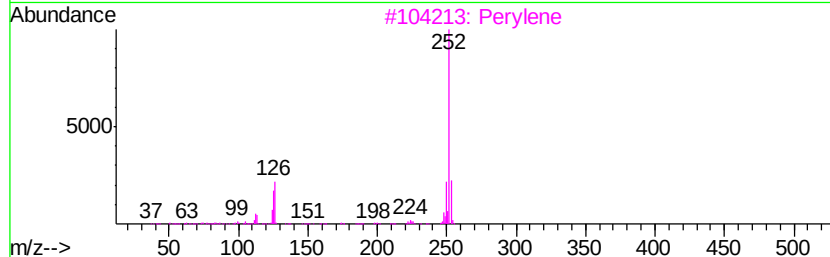
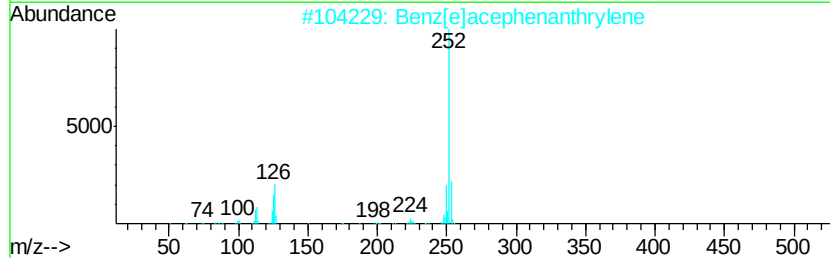
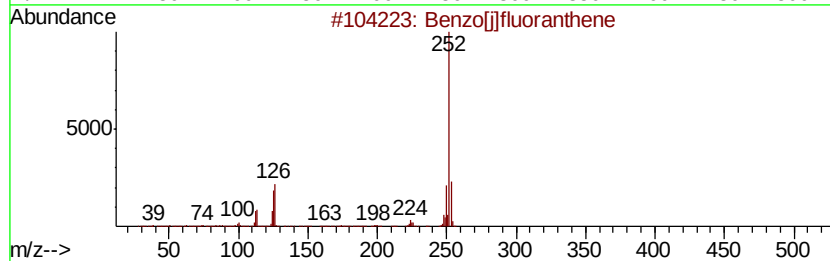
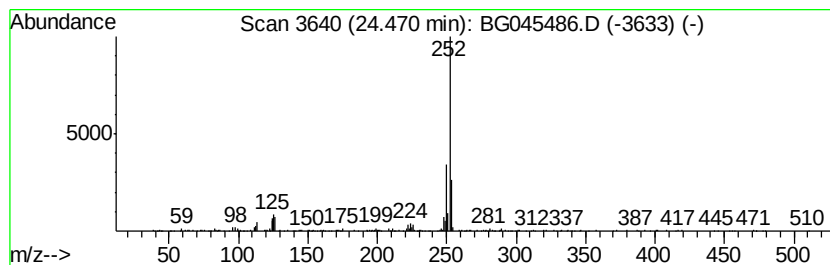
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[j]fluoranthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.47	6.92 ng	516923	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[il]fluoranthene	252	C20H12	000205-82-3	90
2		Benz[el]acephenanthrylene	252	C20H12	000205-99-2	87
3		Perylene	252	C20H12	000198-55-0	81
4		Benzo[elpyrene	252	C20H12	000192-97-2	81
5		Benzo[a]pyrene	252	C20H12	000050-32-8	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045486.D
Acq On : 27 May 2020 21:40
Operator : CG/JU
Sample : L2746-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

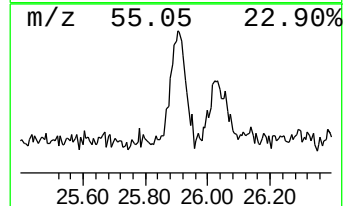
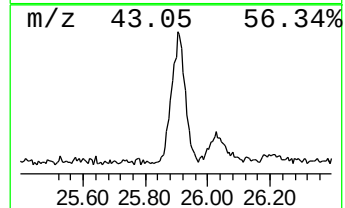
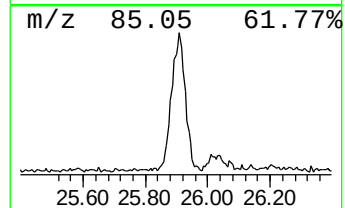
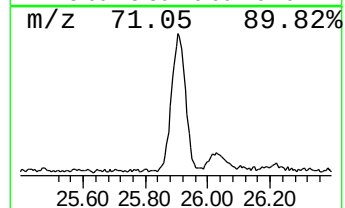
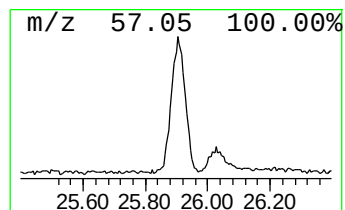
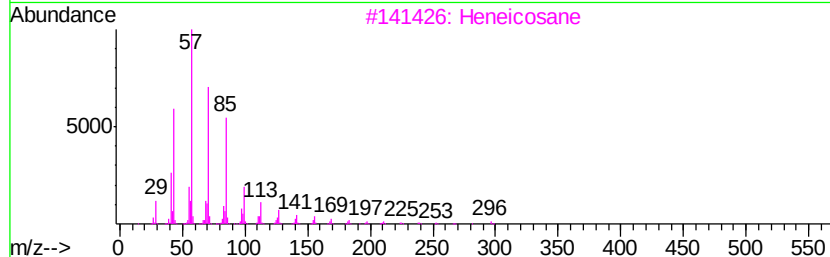
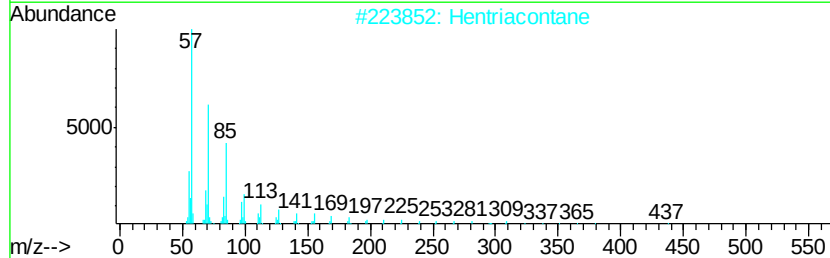
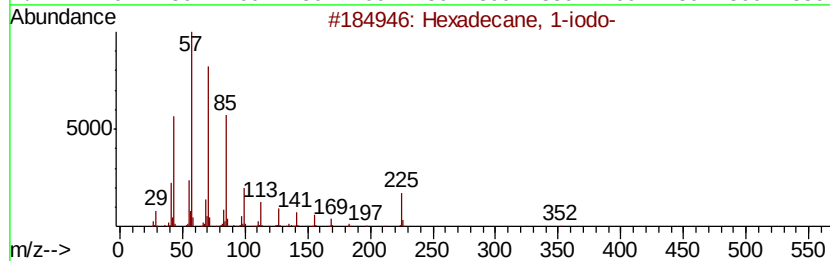
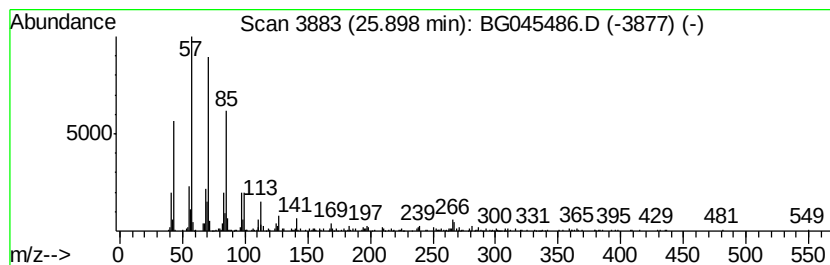
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ClientSampleId :
NM70-COMP-2020-0-6

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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 Hexadecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
25.90	8.46 ng	632211	Perylene-d12		24.76		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Pentacosane	352	C25H52	000629-99-2	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045486.D
Acq On : 27 May 2020 21:40
Operator : CG/JU
Sample : L2746-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

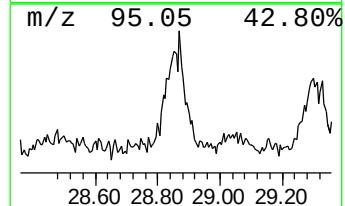
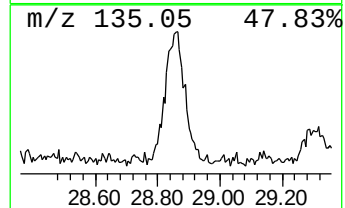
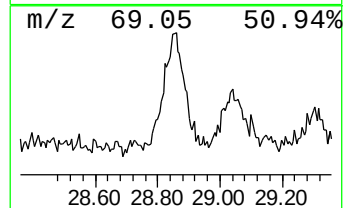
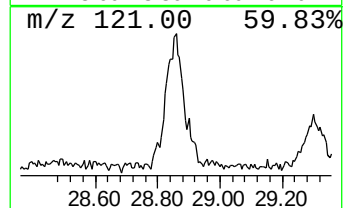
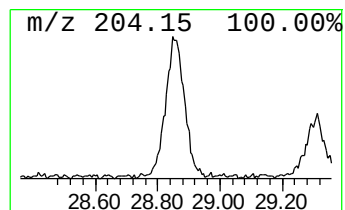
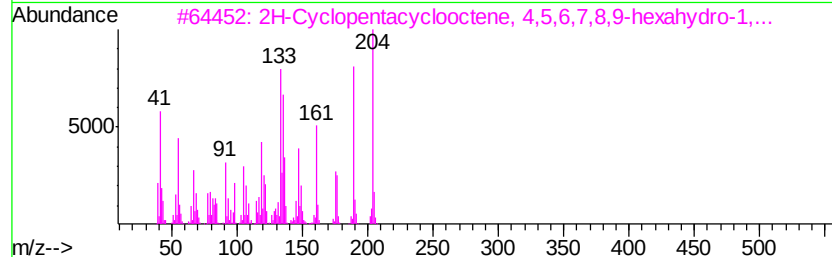
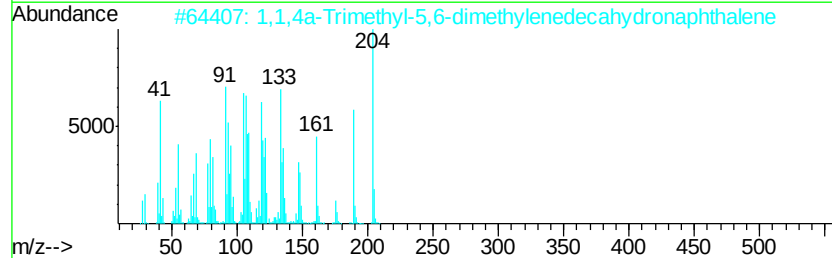
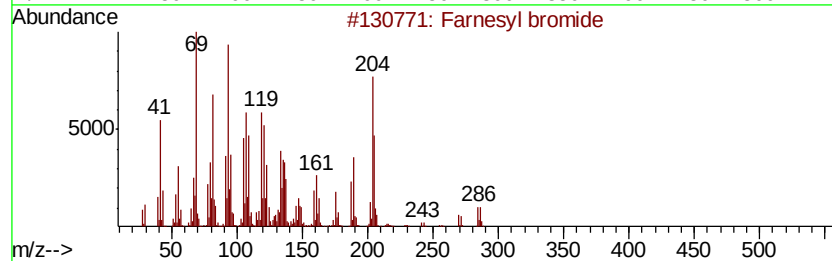
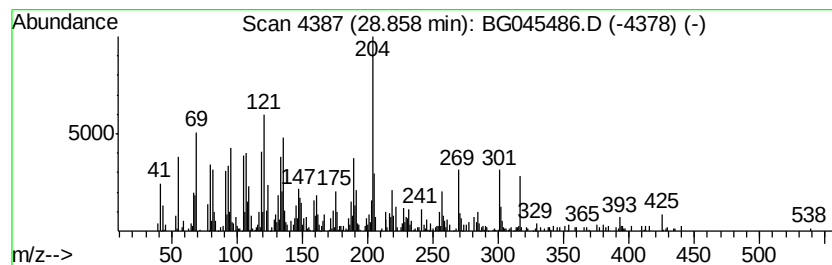
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Farnesyl bromide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.86	17.08 ng	1276420	Perylene-d12	24.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Farnesyl bromide	284 C15H25Br	006874-67-5	50
2	1,1,4a-Trimethyl-5,6-dimethylene...	204 C15H24	1000193-60-8	49
3	2H-Cyclopentacyclooctene, 4,5,6,...	204 C15H24	1000221-85-8	49
4	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204 C14H20O	124957-09-1	43
5	1,2,4,8-Tetramethylbicyclo[6.3.0...	204 C15H24	137235-51-9	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052720\
Data File : BG045486.D
Acq On : 27 May 2020 21:40
Operator : CG/JU
Sample : L2746-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM70-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
5H-Dibenzo[a,d]cy...	18.27	3.3	ng	246280	4	17.35	1514570	20.0
4H-Cyclopenta[def...	18.42	3.2	ng	244113	4	17.35	1514570	20.0
11H-Benzo[b]fluorene	20.26	2.3	ng	245883	5	21.61	2179480	20.0
Bromoacetic acid,...	21.26	4.8	ng	522510	5	21.61	2179480	20.0
Benzo[j]fluoranthene	24.47	6.9	ng	516923	6	24.76	1494230	20.0
Hexadecane, 1-iodo-	25.90	8.5	ng	632211	6	24.76	1494230	20.0
Farnesyl bromide	28.86	17.1	ng	1276420	6	24.76	1494230	20.0