

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
 Data File : BG045560.D
 Acq On : 1 Jun 2020 17:56
 Operator : CG/JU
 Sample : L2792-12
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NM75-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	5.543	410	418	431	rBV	624982	1088722	29.59%	4.135%
2	7.147	680	691	709	rBV	736019	1346541	36.60%	5.114%
3	7.952	820	828	838	rBV	220247	400564	10.89%	1.521%
4	8.275	875	883	893	rBV	694212	1220422	33.17%	4.635%
5	9.109	1017	1025	1044	rBV	515168	1007177	27.37%	3.825%
6	10.760	1298	1306	1319	rBV	298468	586351	15.94%	2.227%
7	13.215	1716	1724	1734	rBV	1586799	2602100	70.72%	9.882%
8	14.044	1858	1865	1875	rBV	150122	240504	6.54%	0.913%
9	14.596	1949	1959	1967	rBV	554685	901625	24.51%	3.424%
10	16.088	2205	2213	2228	rBV	1244096	2023794	55.01%	7.686%
11	17.345	2419	2427	2431	rBV	654132	1051528	28.58%	3.993%
12	17.386	2431	2434	2439	rVB	142191	205405	5.58%	0.780%
13	17.474	2446	2449	2454	rVB2	27985	40717	1.11%	0.155%
14	18.267	2581	2584	2589	rVB2	33615	50265	1.37%	0.191%
15	18.414	2603	2609	2613	rBV4	46025	87482	2.38%	0.332%
16	19.131	2725	2731	2736	rBV2	26377	53741	1.46%	0.204%
17	19.272	2751	2755	2762	rBV6	28415	55078	1.50%	0.209%
18	19.342	2762	2767	2771	rBV	136629	189150	5.14%	0.718%
19	19.395	2771	2776	2782	rVB	367694	529352	14.39%	2.010%
20	19.759	2828	2838	2846	rBV	338889	608808	16.55%	2.312%
21	19.959	2865	2872	2884	rVB	2756901	3679227	100.00%	13.973%
22	20.088	2887	2894	2900	rBV6	34760	87256	2.37%	0.331%
23	20.247	2912	2921	2931	rBV2	62492	168248	4.57%	0.639%
24	20.353	2933	2939	2943	rBV2	36525	61225	1.66%	0.233%
25	20.406	2945	2948	2952	rVB2	36906	56339	1.53%	0.214%
26	20.599	2976	2981	2984	rBV2	36164	53106	1.44%	0.202%
27	21.011	3046	3051	3057	rVB3	35217	58449	1.59%	0.222%
28	21.263	3090	3094	3103	rVB4	141290	274454	7.46%	1.042%
29	21.604	3143	3152	3157	rBV2	694518	1503782	40.87%	5.711%
30	21.645	3157	3159	3173	rVB	179745	296350	8.05%	1.125%
31	21.798	3181	3185	3191	rBV3	40623	68489	1.86%	0.260%
32	22.403	3283	3288	3296	rBV7	55685	139234	3.78%	0.529%
33	23.413	3458	3460	3468	rVB5	63230	104996	2.85%	0.399%
34	23.754	3510	3518	3525	rBV2	148739	464254	12.62%	1.763%

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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	23.866	3533	3537	3543	rVB	134514	250517	6.81%	0.951%
36	23.930	3543	3548	3556	rBV6	64116	149867	4.07%	0.569%
37	24.459	3632	3638	3647	rVB	84662	224705	6.11%	0.853%
38	24.594	3655	3661	3671	rVB	115420	308290	8.38%	1.171%
39	24.753	3678	3688	3708	rBV2	396329	1234122	33.54%	4.687%
40	25.293	3772	3780	3790	rVB9	70152	204787	5.57%	0.778%
41	25.892	3873	3882	3893	rVB	329363	1036005	28.16%	3.934%
42	26.027	3895	3905	3923	rBV6	97738	450283	12.24%	1.710%
43	28.307	4287	4293	4295	rBV3	35872	75400	2.05%	0.286%
44	28.835	4365	4383	4404	rBV3	139902	837824	22.77%	3.182%
45	29.288	4449	4460	4473	rBV3	54793	255351	6.94%	0.970%

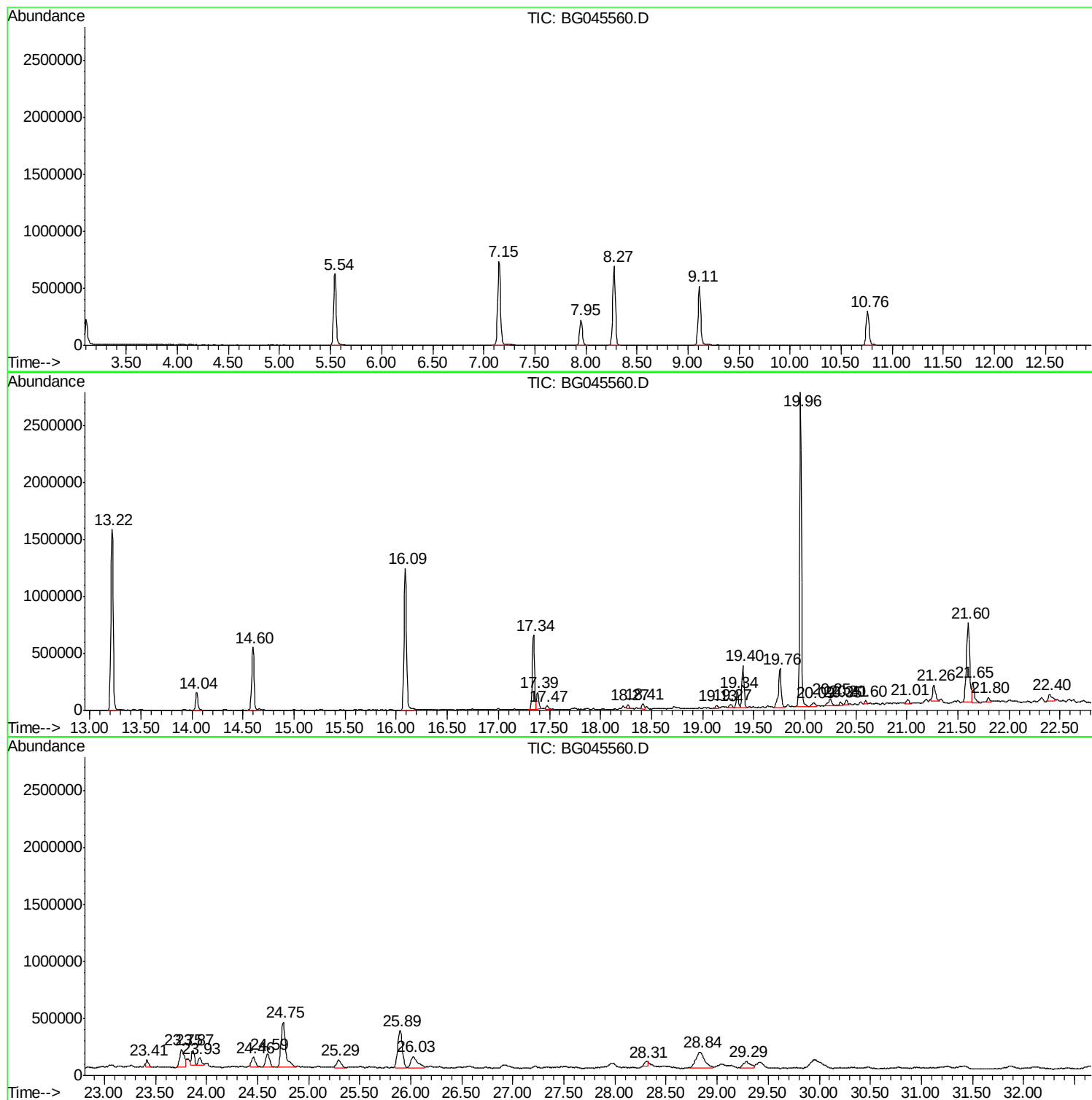
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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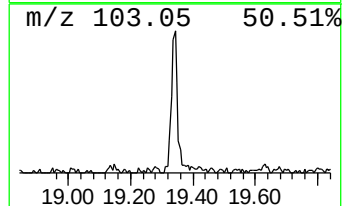
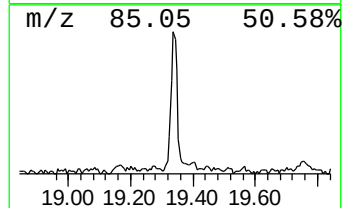
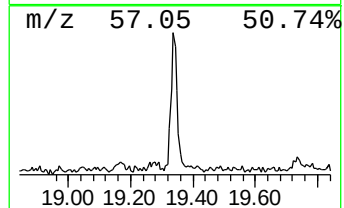
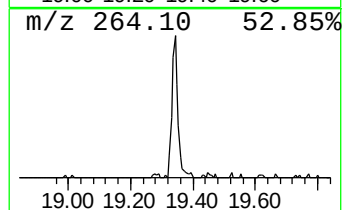
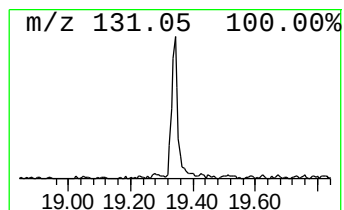
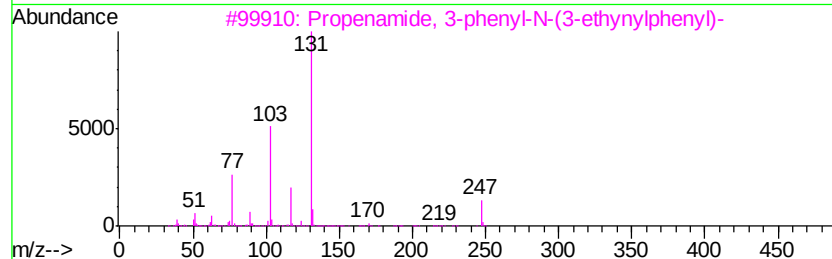
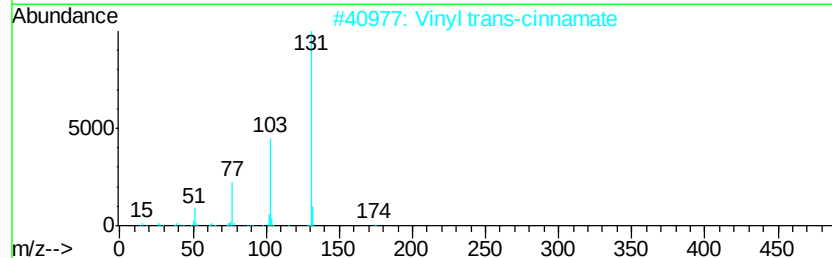
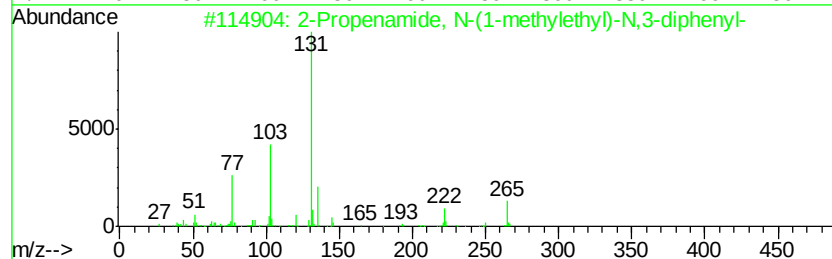
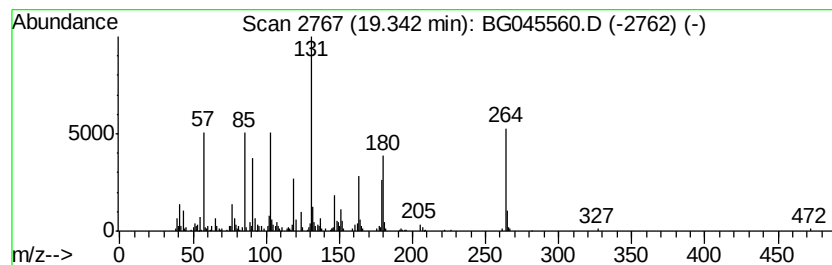
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TIC Library : C:\Database\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 2 unknown19.34 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	3.60 ng	189150	Phenanthrene-d10	17.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	30
2		Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	22
3		Propenamide, 3-phenyl-N-(3-ethyn...	247	C17H13NO	294667-02-0	22
4		1-Penten-3-one, 4-methyl-1-phenyl-	174	C12H14O	003160-32-5	22
5		Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	22



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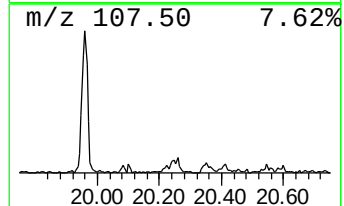
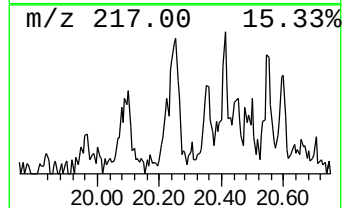
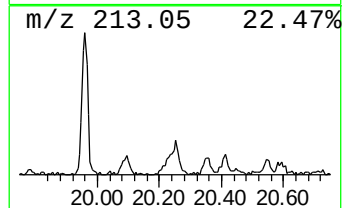
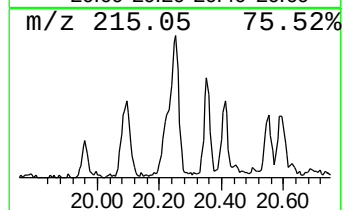
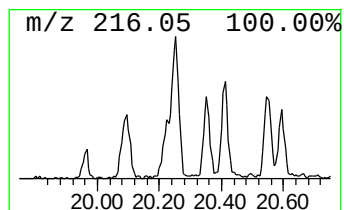
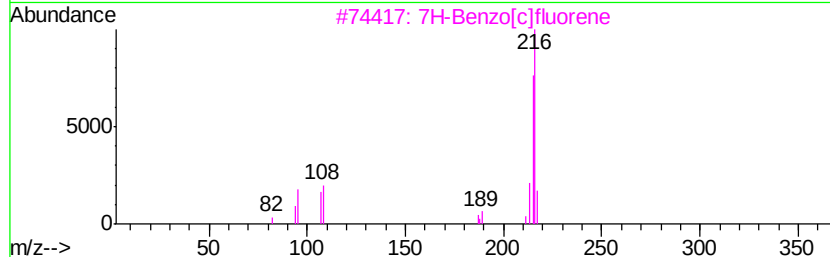
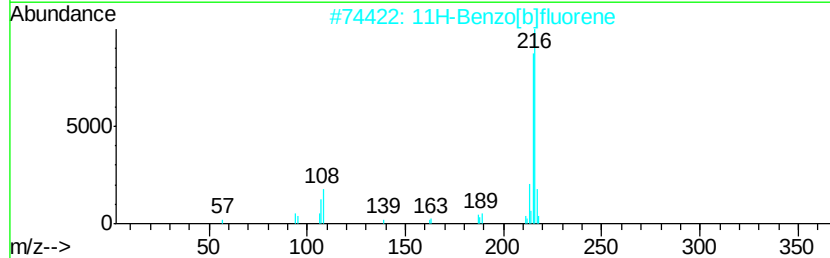
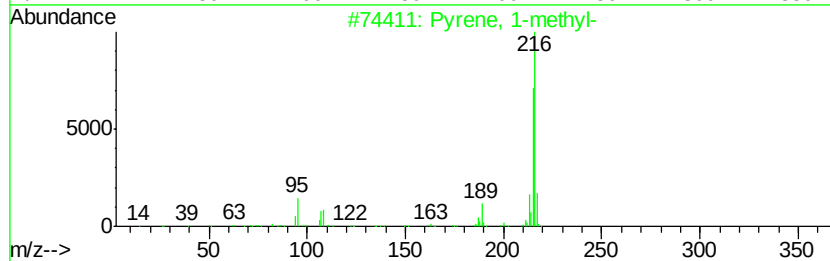
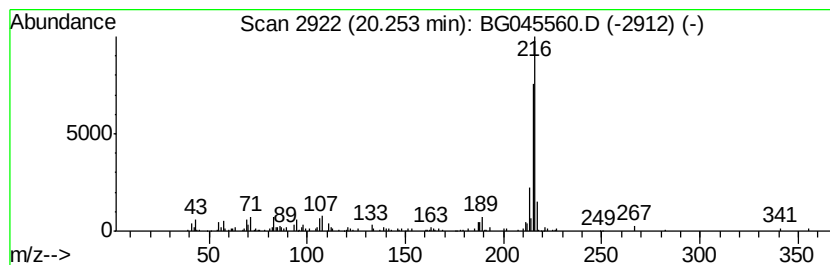
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.25	2.24 ng	168248	Chrysene-d12	21.60
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyrene, 1-methyl-	216 C17H12	002381-21-7 90
2		11H-Benzo[b]fluorene	216 C17H12	000243-17-4 90
3		7H-Benzo[c]fluorene	216 C17H12	000205-12-9 87
4		Fluoranthene, 2-methyl-	216 C17H12	033543-31-6 83
5		11H-Benzo[a]fluorene	216 C17H12	000238-84-6 83



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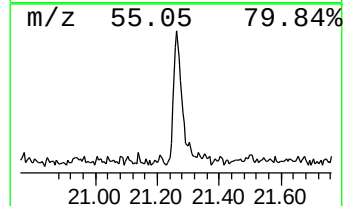
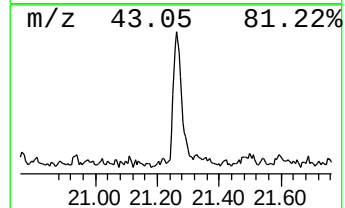
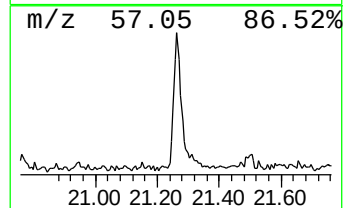
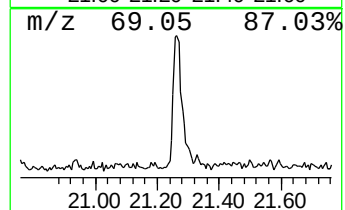
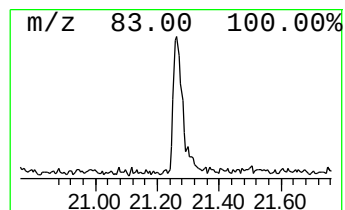
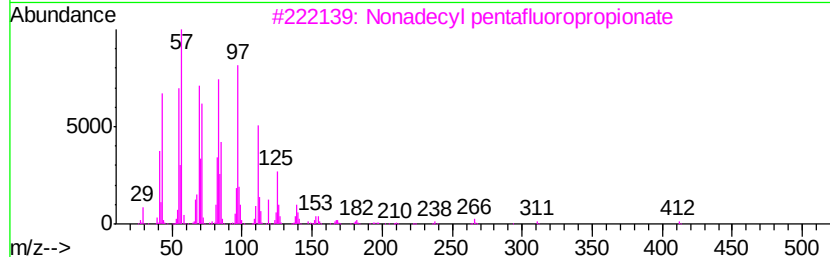
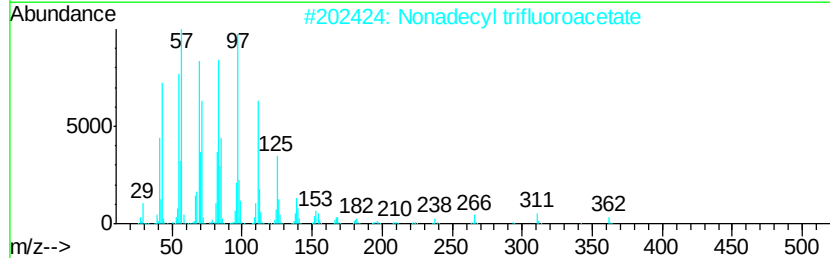
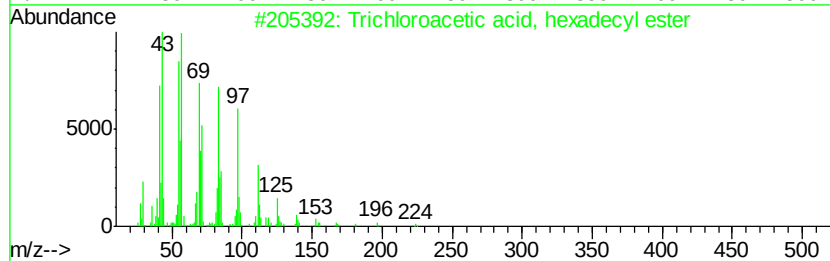
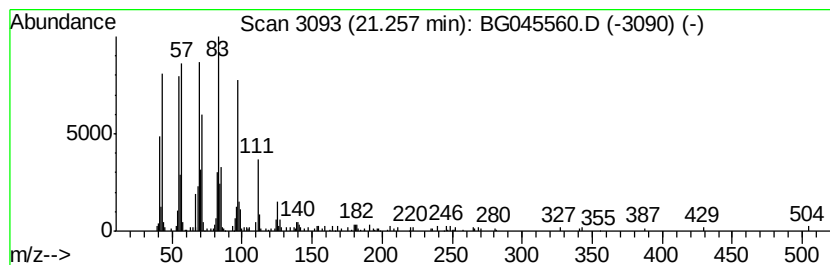
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	3.65 ng	274454	Chrysene-d12	21.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	81
4		Cyclooctacosane	392	C28H56	000297-24-5	81
5		Cyclotetracosane	336	C24H48	000297-03-0	74



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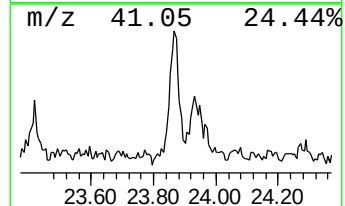
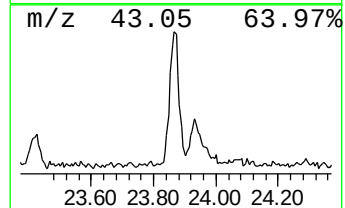
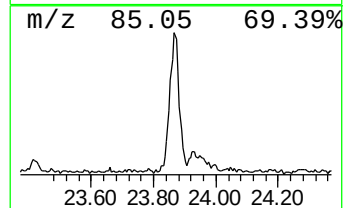
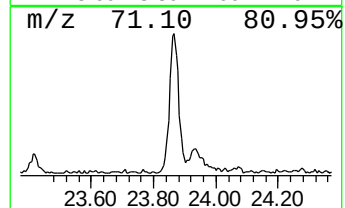
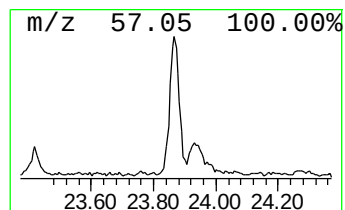
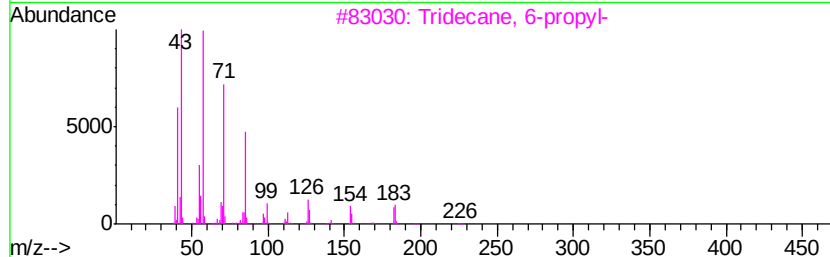
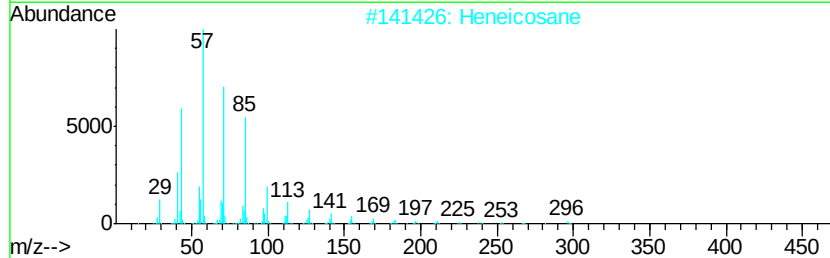
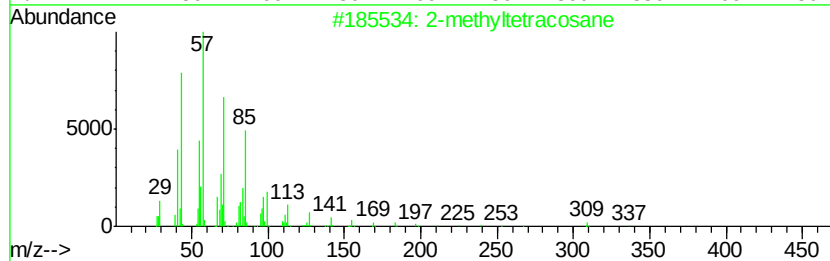
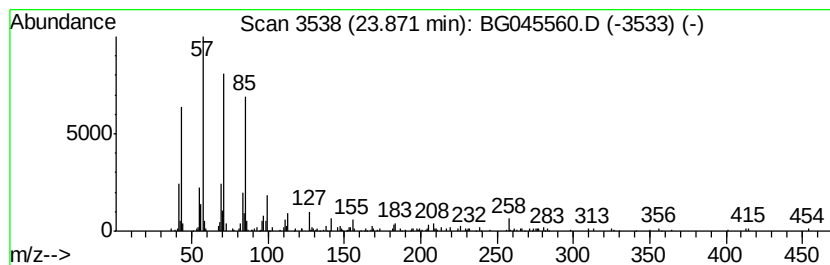
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 2-methyltetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	4.06 ng	250517	Perylene-d12	24.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyltetracosane		352	C25H52	1000376-72-6	86
2	Heneicosane		296	C21H44	000629-94-7	83
3	Tridecane, 6-propyl-		226	C16H34	055045-10-8	64
4	Sulfurous acid, nonyl 2-propyl e...		250	C12H26O3S	1000309-12-0	64
5	Heptacosane		380	C27H56	000593-49-7	58



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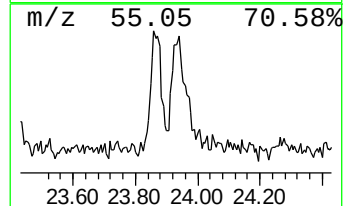
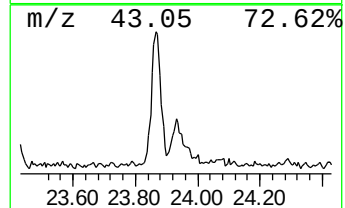
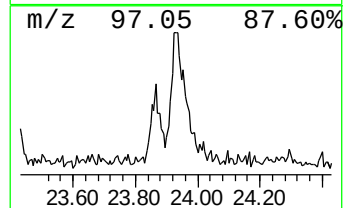
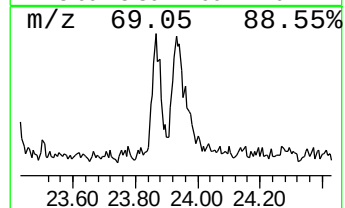
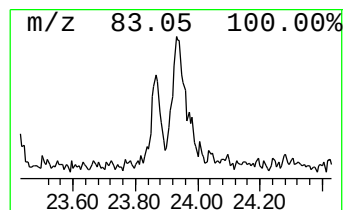
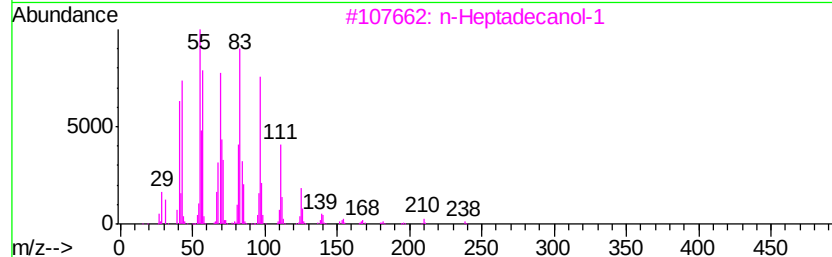
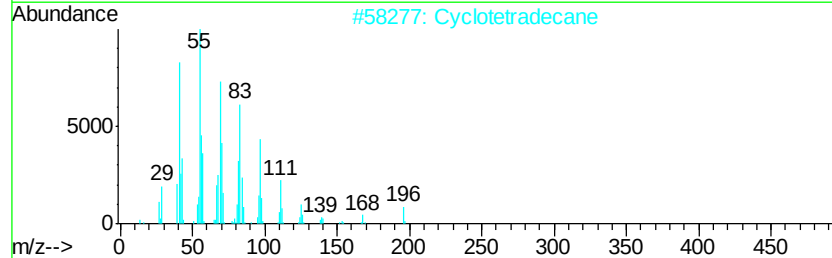
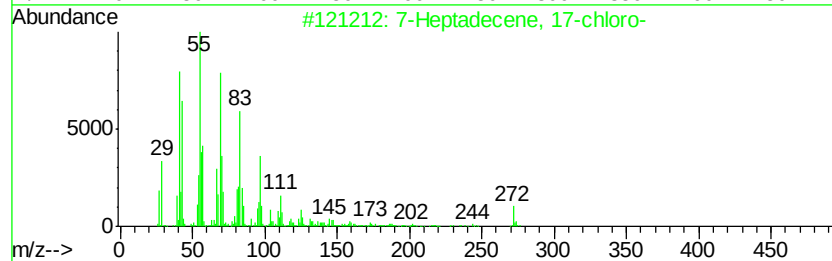
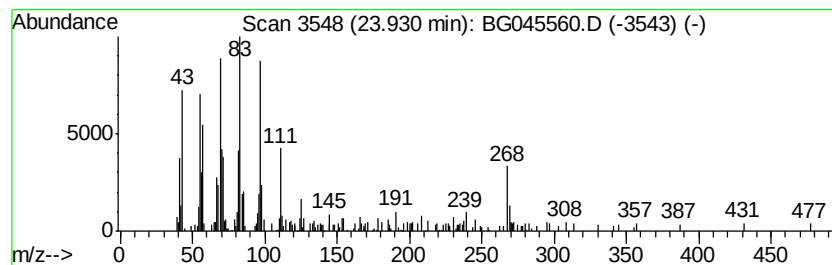
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 7-Heptadecene, 17-chloro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.93	2.43 ng	149867	Perylene-d12	24.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Heptadecene, 17-chloro-	272	C17H33Cl	056554-79-1	89
2	Cyclotetradecane	196	C14H28	000295-17-0	89
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	86
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045560.D
Acq On : 1 Jun 2020 17:56
Operator : CG/JU
Sample : L2792-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

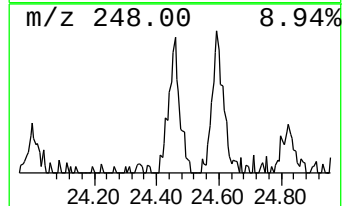
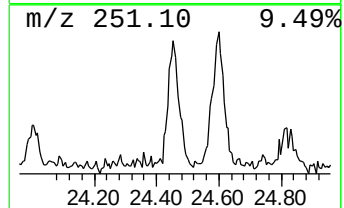
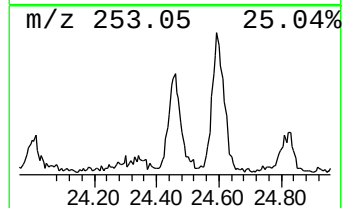
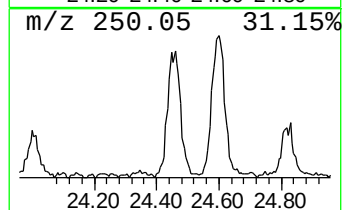
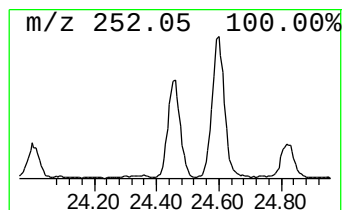
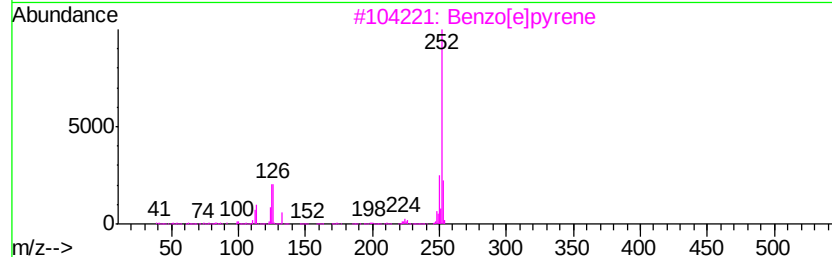
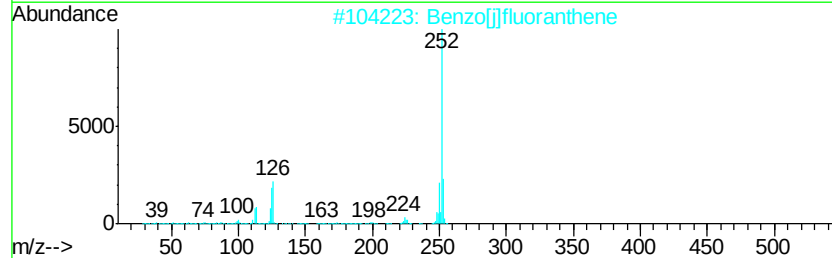
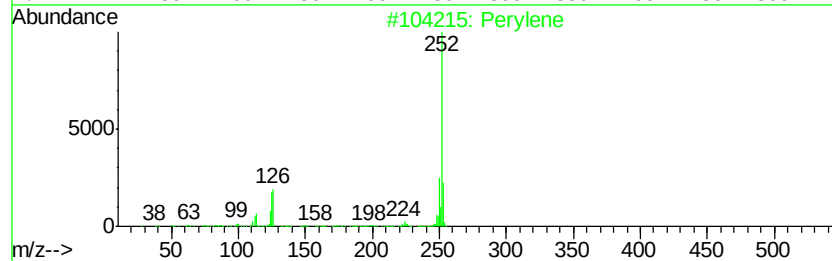
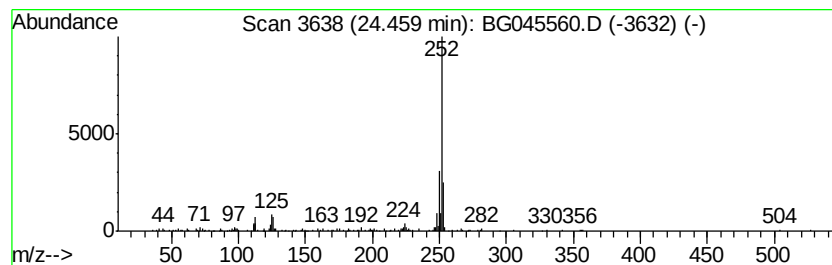
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
24.46	3.64 ng	224705	Perylene-d12		24.75
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[il]fluoranthene	252	C20H12	000205-82-3	76
3	Benzo[elpvrene	252	C20H12	000192-97-2	76
4	Benz[elacephenanthrylene	252	C20H12	000205-99-2	76
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
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Sample : L2792-12
Misc :
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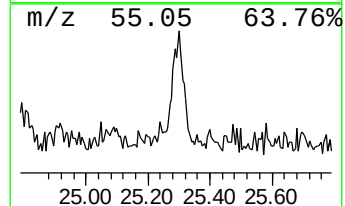
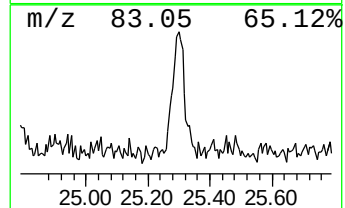
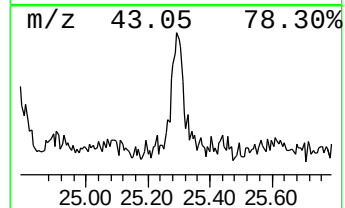
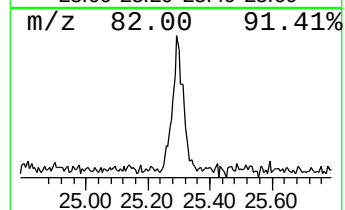
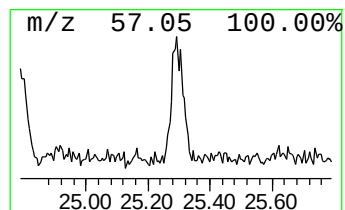
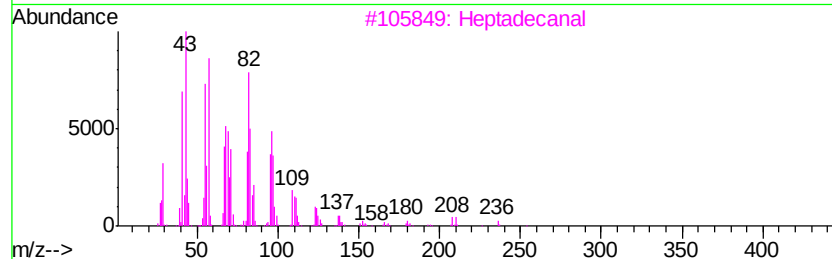
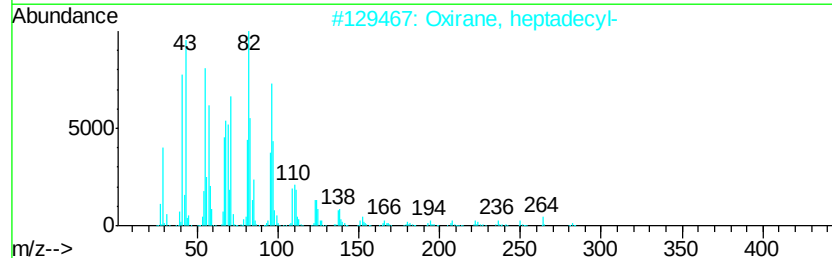
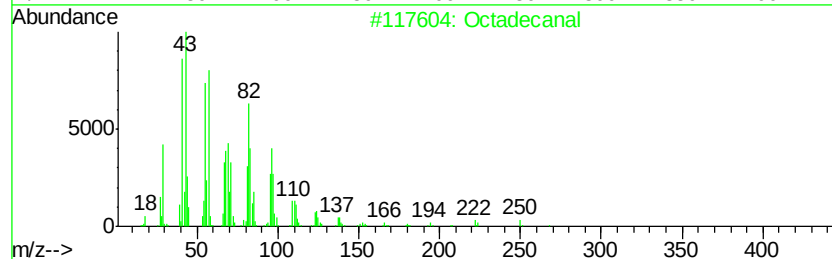
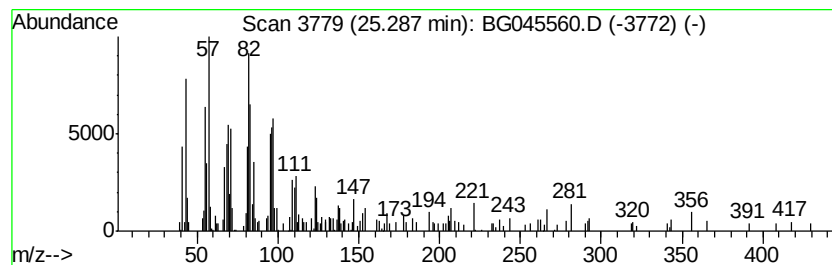
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.29	3.32 ng	204787	Perylene-d12	24.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	89
3	Heptadecanal	254	C17H34O	1000376-70-0	83
4	Disparlure	282	C19H38O	029804-22-6	80
5	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
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Operator : CG/JU
Sample : L2792-12
Misc :
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Instrument :
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ClientSampleId :
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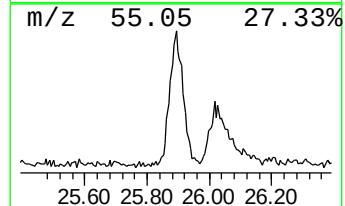
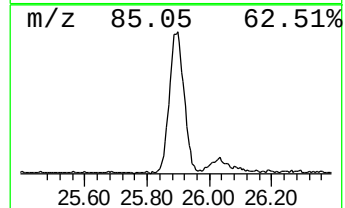
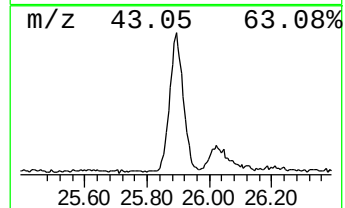
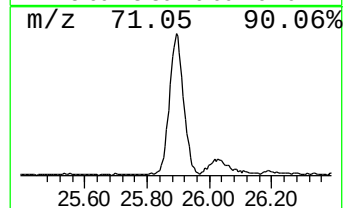
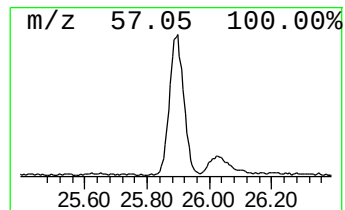
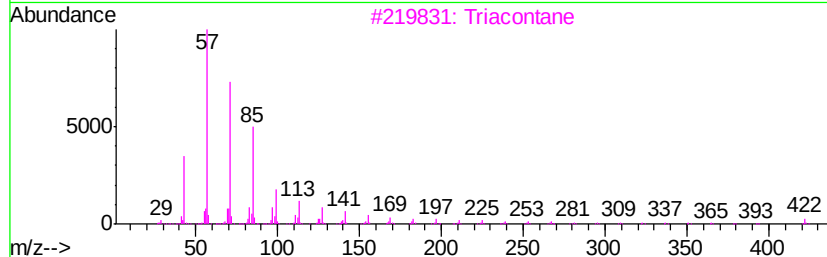
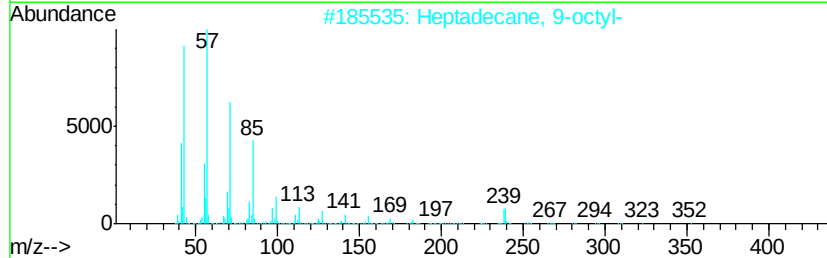
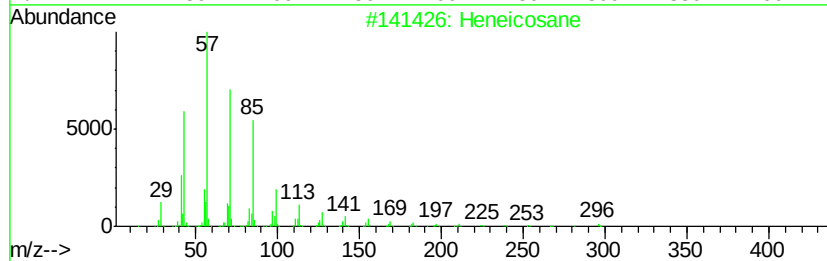
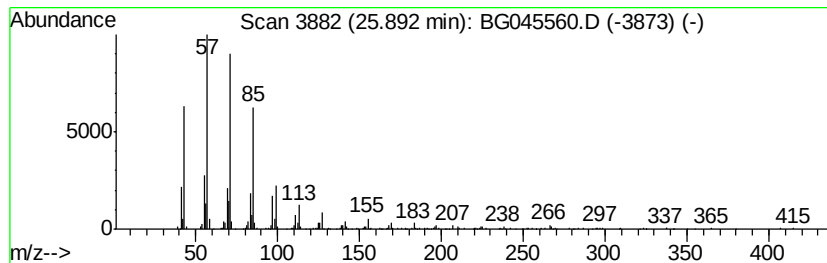
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.89	16.79 ng	1036010	Perylene-d12	24.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90
3	Triacontane		422	C30H62	000638-68-6	87
4	Hexacosane		366	C26H54	000630-01-3	87
5	Octadecane		254	C18H38	000593-45-3	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
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Sample : L2792-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

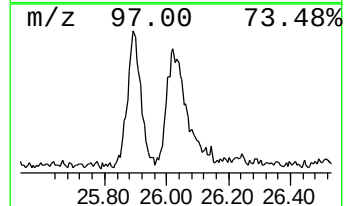
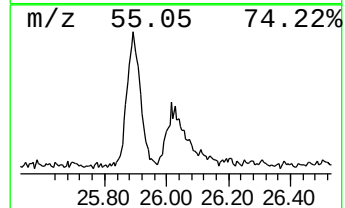
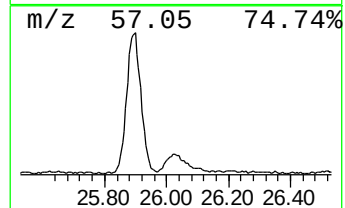
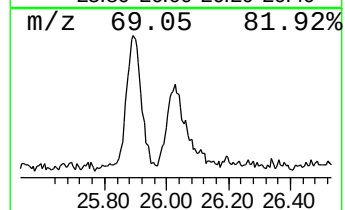
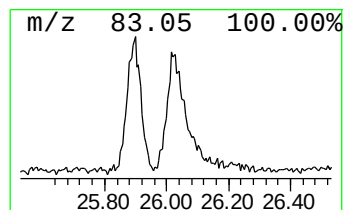
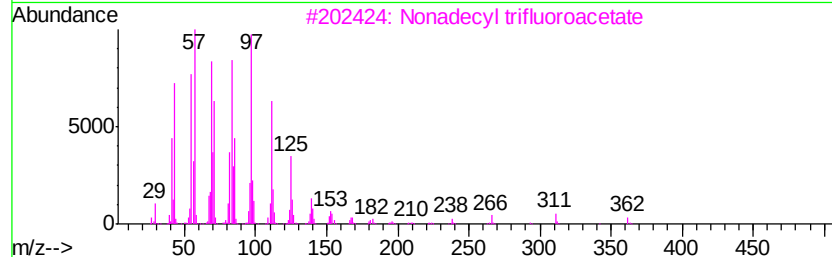
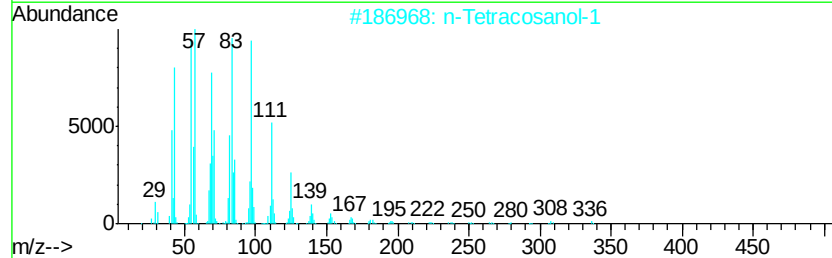
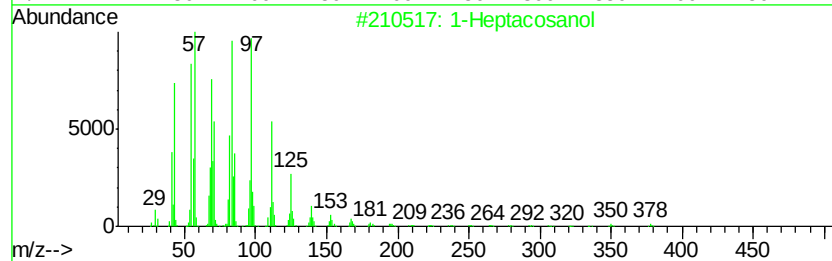
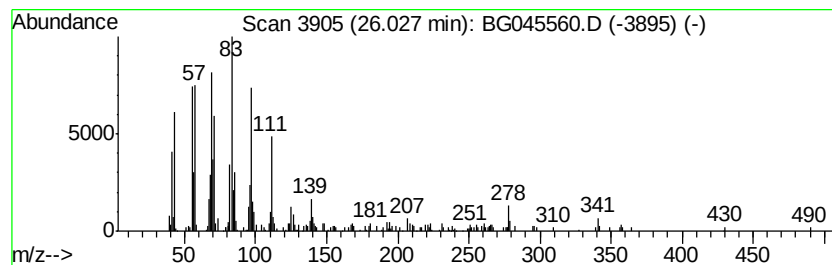
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.03	7.30 ng	450283	Perylene-d12	24.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	83
4	Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	70
5	Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	55



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
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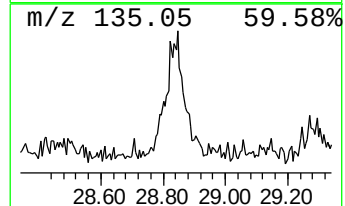
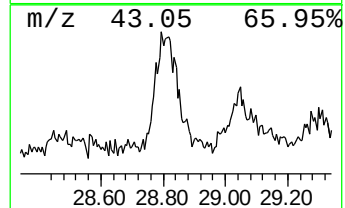
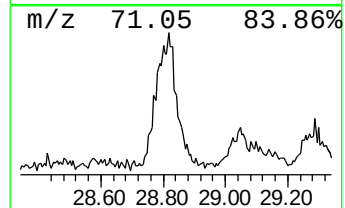
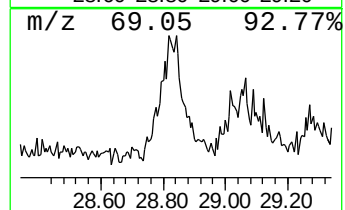
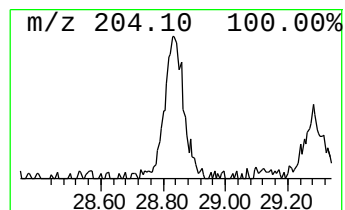
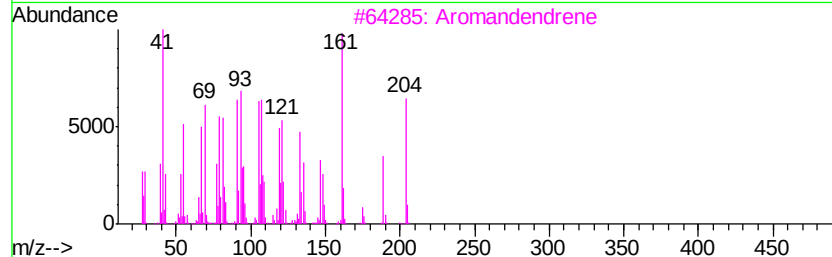
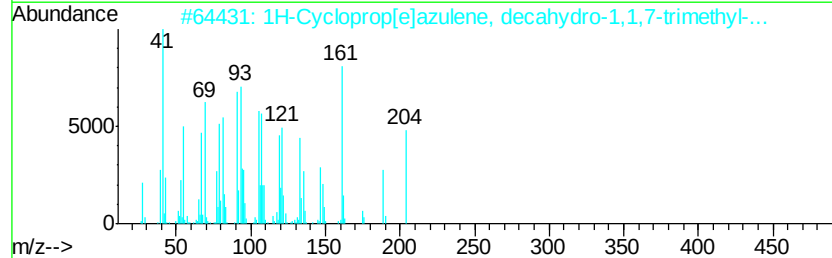
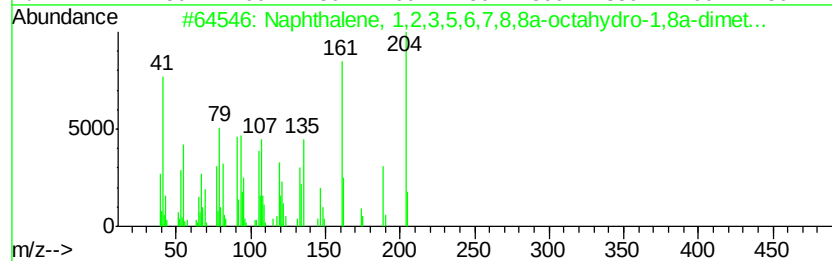
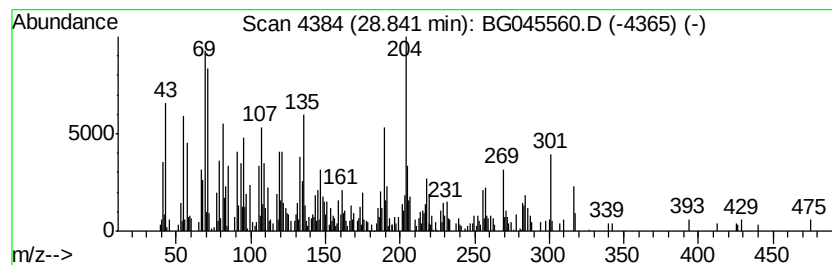
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Naphthalene, 1,2,3,5,6,7,8,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.84	13.58 ng	837824	Perylene-d12	24.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204 C15H24	004630-07-3 86
2		1H-Cycloprop[elazulene, decahydr...	204 C15H24	072747-25-2 83
3		Aromandendrene	204 C15H24	000489-39-4 78
4		Farnesyl bromide	284 C15H25Br	006874-67-5 60
5		Naphthalene, decahydro-4a-methyl...	204 C15H24	017066-67-0 50



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045560.D
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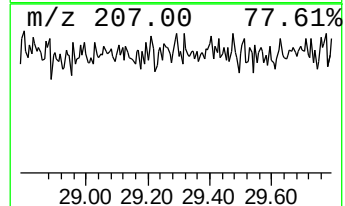
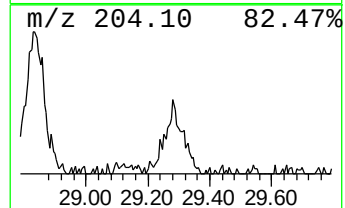
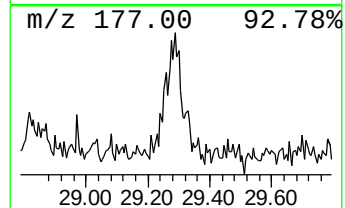
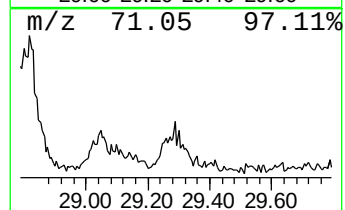
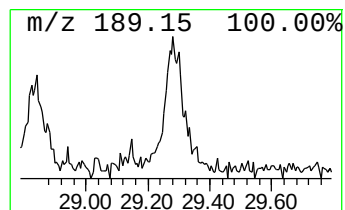
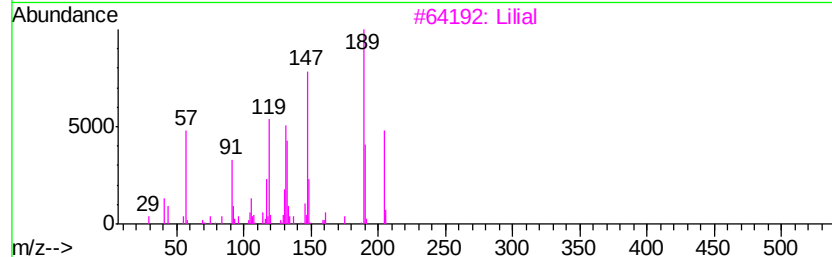
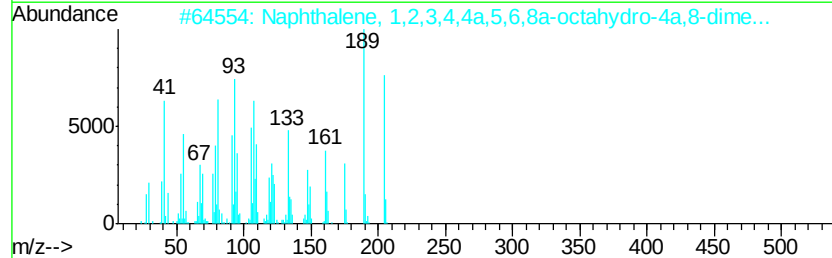
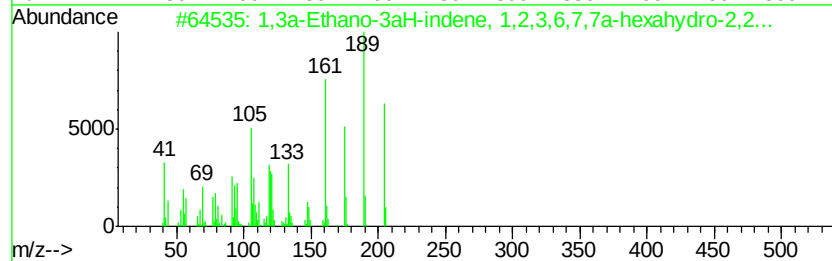
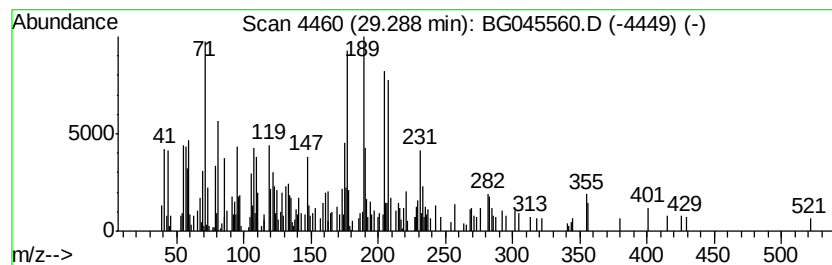
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown29.29 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.29	4.14 ng	255351	Perylene-d12	24.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	38
2		Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	38
3		Lilial	204	C14H20O	000080-54-6	38
4		2H-1,3-Oxazine, 2-[(2,6-dimethyl...	204	C12H16N2O	054708-09-7	30
5		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG060120\
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 Misc :
 ALS Vial : 8 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pyrene, 1-methyl-	20.25	2.2 ng		168248	5	21.60	1503780	20.0
Trichloroacetic a...	21.26	3.6 ng		274454	5	21.60	1503780	20.0
2-methyltetracosane	23.87	4.1 ng		250517	6	24.75	1234120	20.0
7-Heptadecene, 17...	23.93	2.4 ng		149867	6	24.75	1234120	20.0
Perylene	24.46	3.6 ng		224705	6	24.75	1234120	20.0
Octadecanal	25.29	3.3 ng		204787	6	24.75	1234120	20.0
Heneicosane	25.89	16.8 ng		1036010	6	24.75	1234120	20.0
1-Heptacosanol	26.03	7.3 ng		450283	6	24.75	1234120	20.0
Naphthalene, 1,2,...	28.84	13.6 ng		837824	6	24.75	1234120	20.0
unknown29.29	29.29	4.1 ng		255351	6	24.75	1234120	20.0