

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
 Data File : BM029034.D
 Acq On : 09 Mar 2021 00:22
 Operator : CG/JU
 Sample : M1589-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FK-GF-02-067-B

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029034.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	379	384	395	rBB	192281	272546	58.19%	7.819%
2	6.869	654	660	671	rBV	175598	278940	59.55%	8.003%
3	7.669	791	796	802	rBB	45223	65875	14.06%	1.890%
4	8.845	989	996	1007	rVB	111955	179459	38.31%	5.149%
5	10.463	1264	1271	1278	rBV	53701	85620	18.28%	2.456%
6	12.951	1688	1694	1701	rVB	248963	344567	73.56%	9.885%
7	13.804	1834	1839	1843	rBB	3970	4819	1.03%	0.138%
8	14.216	1902	1909	1918	rBV3	6240	16603	3.54%	0.476%
9	14.339	1924	1930	1936	rVB	71510	101721	21.72%	2.918%
10	15.833	2179	2184	2191	rVB	182951	251126	53.61%	7.205%
11	17.086	2391	2397	2400	rBV	84116	111422	23.79%	3.197%
12	17.127	2400	2404	2409	rVB	50639	67851	14.49%	1.947%
13	17.215	2415	2419	2425	rVB	10699	14347	3.06%	0.412%
14	17.957	2541	2545	2546	rBV	6391	8042	1.72%	0.231%
15	17.980	2546	2549	2557	rVB2	28739	45507	9.72%	1.306%
16	18.151	2573	2578	2581	rBV2	7917	13280	2.84%	0.381%
17	18.186	2581	2584	2588	rVB2	4454	5830	1.24%	0.167%
18	18.457	2626	2630	2634	rBV2	4187	5698	1.22%	0.163%
19	18.509	2634	2639	2643	rBV2	4574	5395	1.15%	0.155%
20	18.874	2697	2701	2705	rBV	4102	4853	1.04%	0.139%
21	19.027	2721	2727	2731	rBV2	3566	6117	1.31%	0.175%
22	19.139	2739	2746	2751	rBV	87783	110458	23.58%	3.169%
23	19.262	2763	2767	2771	rBV3	10359	12289	2.62%	0.353%
24	19.474	2798	2803	2804	rBV	13421	16175	3.45%	0.464%
25	19.503	2804	2808	2817	rVV	73754	100366	21.43%	2.879%
26	19.580	2817	2821	2826	rVB4	3874	5646	1.21%	0.162%
27	19.709	2836	2843	2848	rBV	416411	468395	100.00%	13.438%
28	19.827	2858	2863	2871	rBV5	5240	12128	2.59%	0.348%
29	19.998	2883	2892	2898	rVB3	10903	24523	5.24%	0.704%
30	20.103	2906	2910	2912	rBV	5550	6649	1.42%	0.191%
31	20.156	2914	2919	2923	rVV2	7577	12440	2.66%	0.357%
32	20.292	2939	2942	2946	rBV	5832	7998	1.71%	0.229%
33	20.345	2946	2951	2955	rVV2	6560	11149	2.38%	0.320%
34	20.745	3016	3019	3024	rBV	9011	13452	2.87%	0.386%
35	20.903	3043	3046	3050	rBV2	9727	13385	2.86%	0.384%
36	20.945	3051	3053	3054	rVV2	8781	7714	1.65%	0.221%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.974	3054	3058	3065	rVV3	63793	93909	20.05%	2.694%
38	21.045	3067	3070	3075	rVB	8445	12504	2.67%	0.359%
39	21.256	3100	3106	3110	rBV2	136863	220776	47.13%	6.334%
40	21.292	3110	3112	3117	rVB	41781	49463	10.56%	1.419%
41	21.845	3204	3206	3212	rVB6	18863	24565	5.24%	0.705%
42	22.774	3360	3364	3378	rVB	44462	136369	29.11%	3.912%
43	23.233	3439	3442	3448	rVB	23135	33857	7.23%	0.971%
44	23.321	3453	3457	3463	rVB	40041	65661	14.02%	1.884%
45	23.415	3468	3473	3478	rBV2	80826	136166	29.07%	3.906%

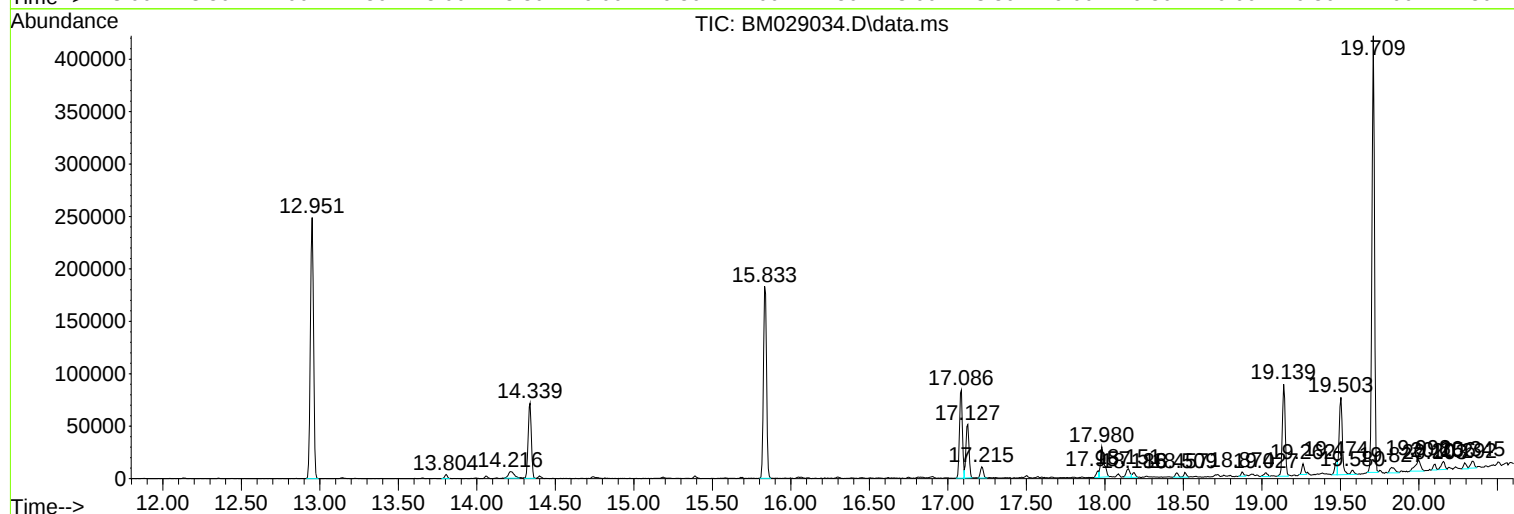
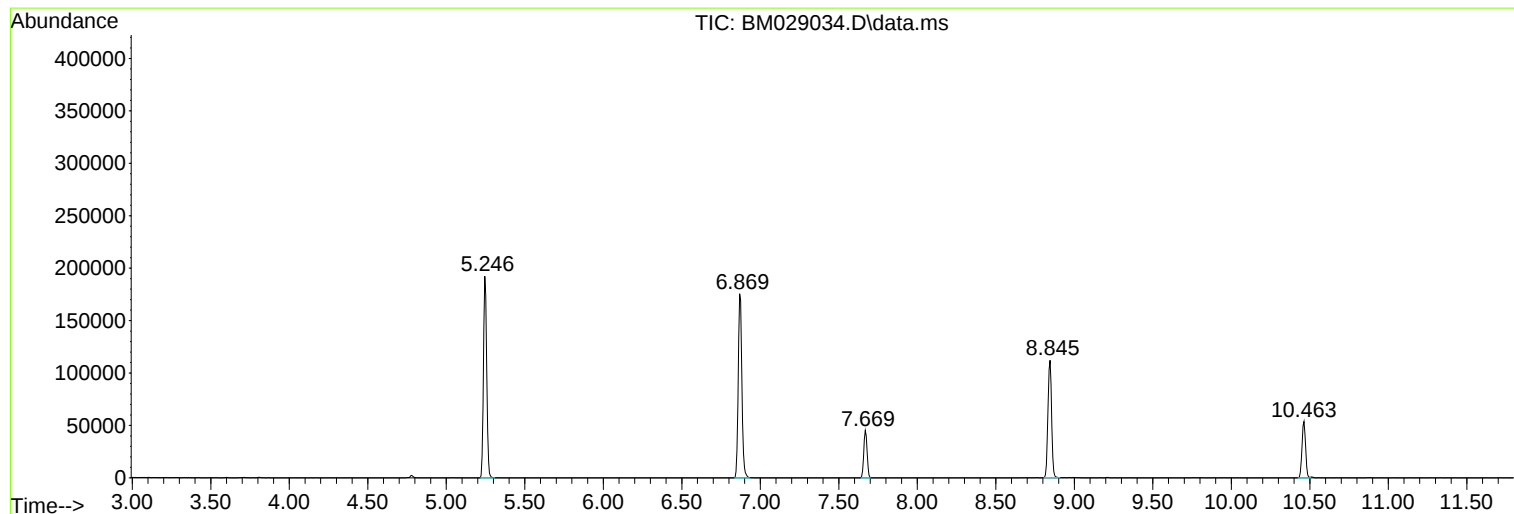
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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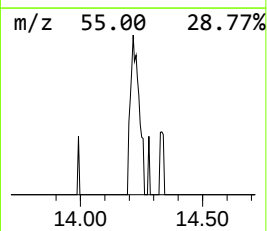
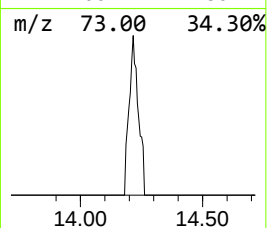
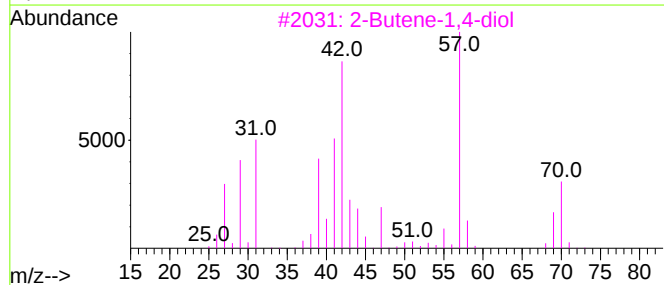
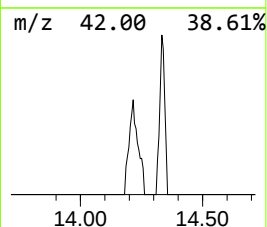
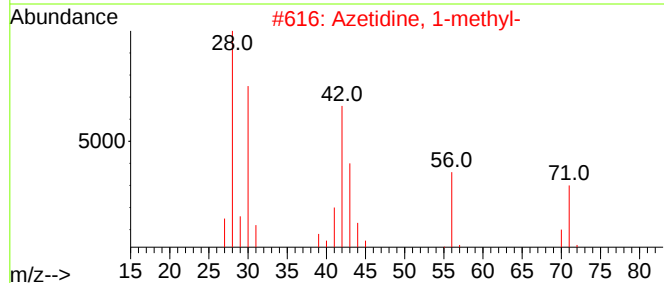
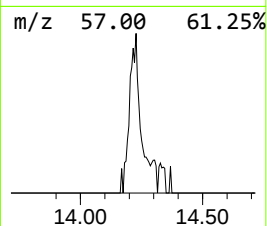
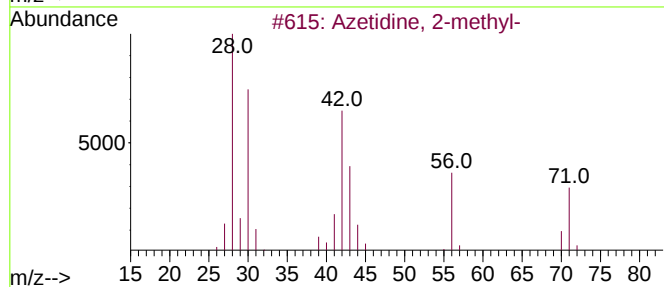
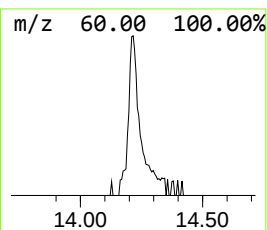
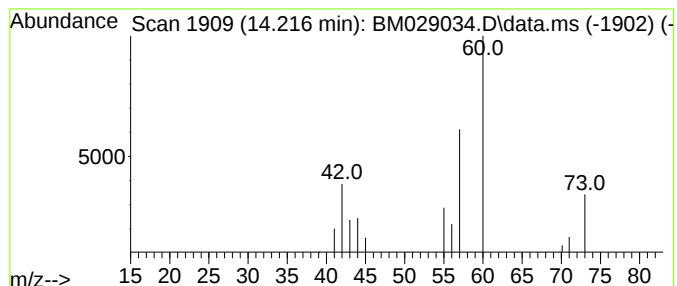
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown14.216 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	3.26 ng	16603	Acenaphthene-d10	14.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	9
2			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	9
3			2-Butene-1,4-diol	88	C4H8O2	000110-64-5	9
4			Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9
5			Butanoic acid	88	C4H8O2	000107-92-6	9



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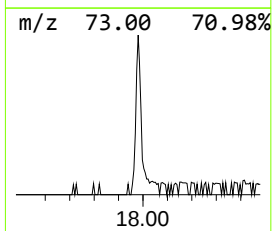
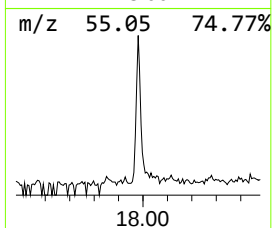
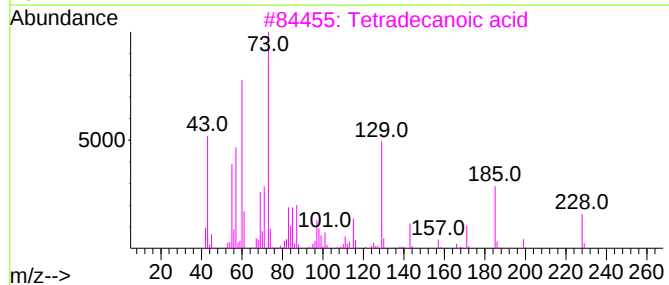
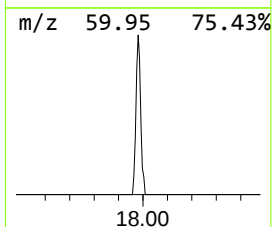
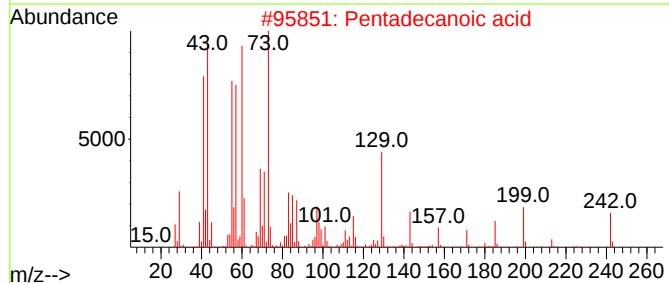
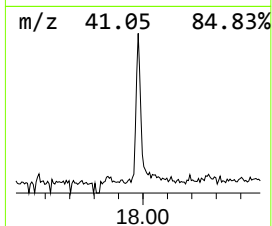
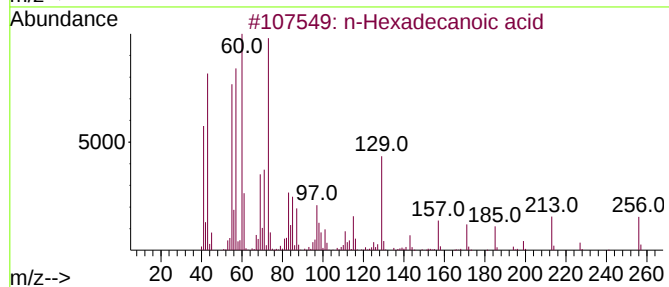
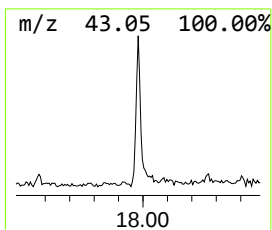
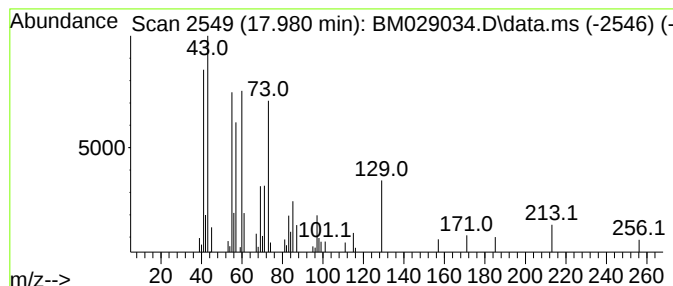
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.980	8.17 ng	45507	Phenanthrene-d10	17.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	53
5			Undecanoic acid	186	C11H22O2	000112-37-8	47



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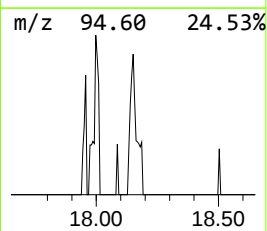
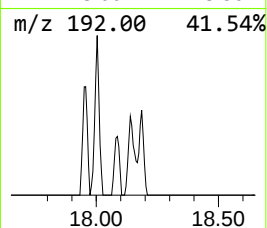
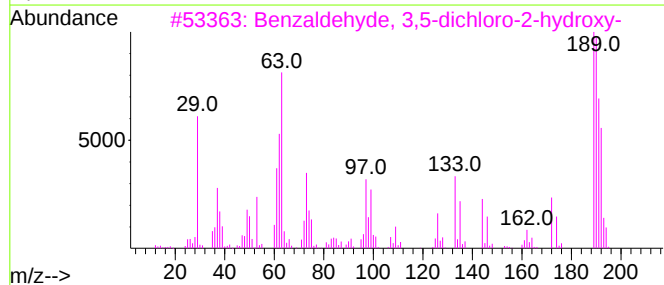
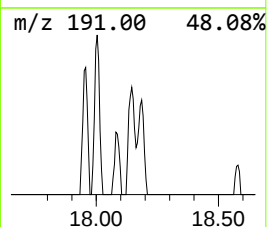
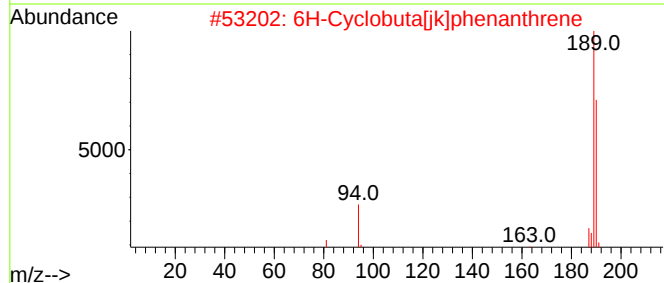
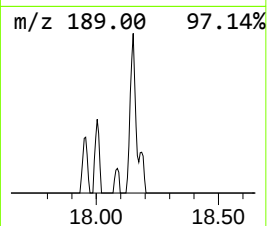
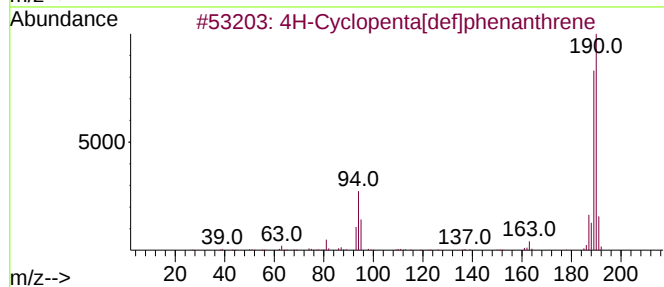
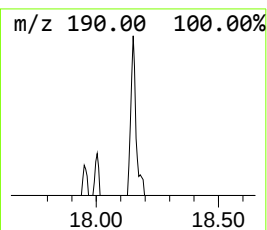
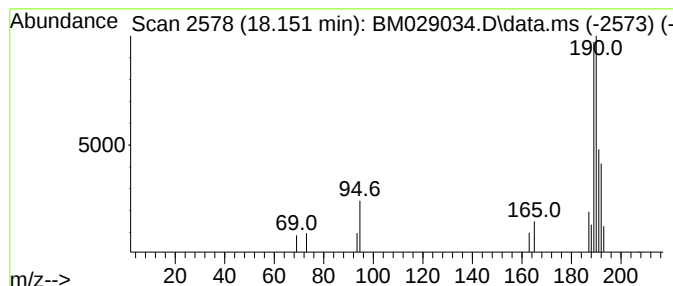
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	2.38 ng	13280	Phenanthrene-d10	17.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
3			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	45
4			2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5			Methyl diselenide	190	C2H6Se2	007101-31-7	35



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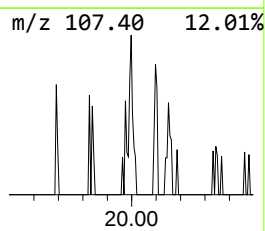
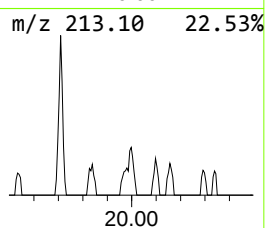
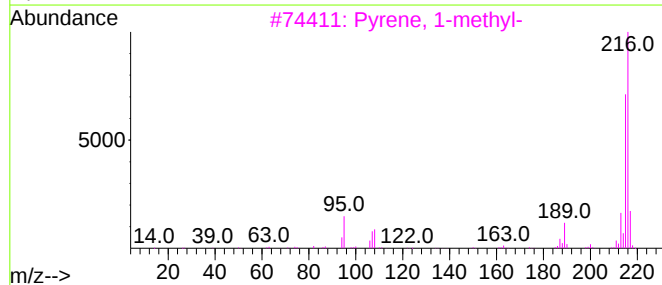
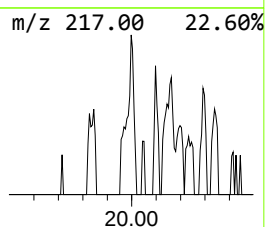
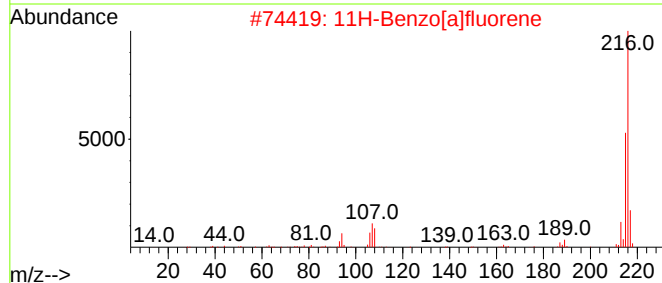
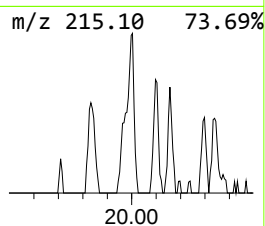
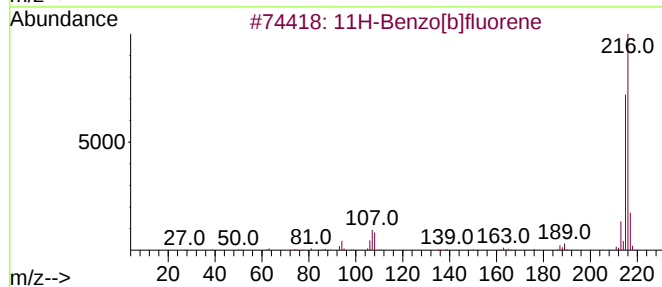
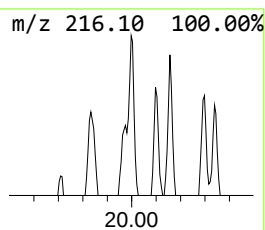
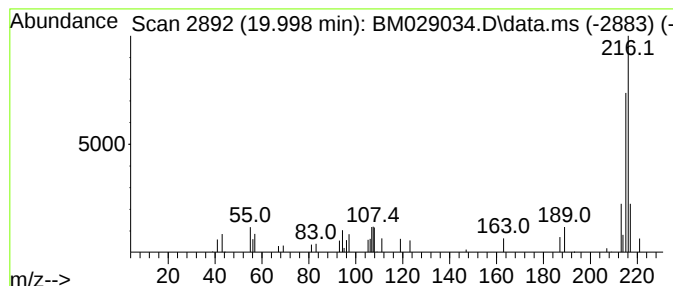
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 11H-Benzo[b]fluorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.998	2.22 ng	24523	Chrysene-d12	21.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3			Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
4			Pyrene, 2-methyl-	216	C17H12	003442-78-2	80
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	72



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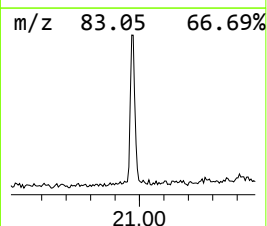
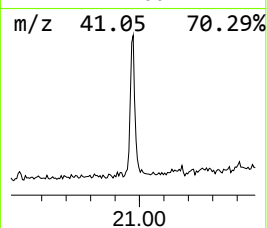
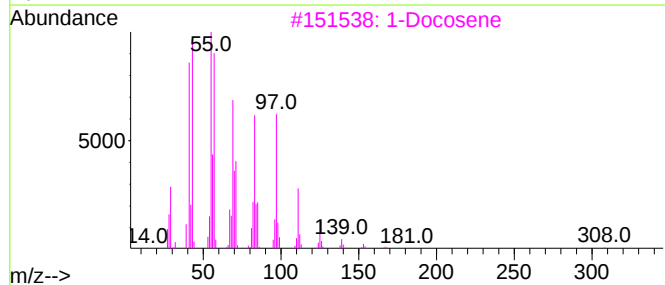
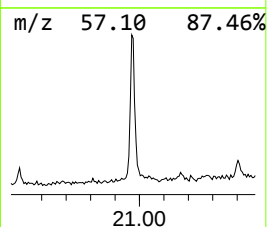
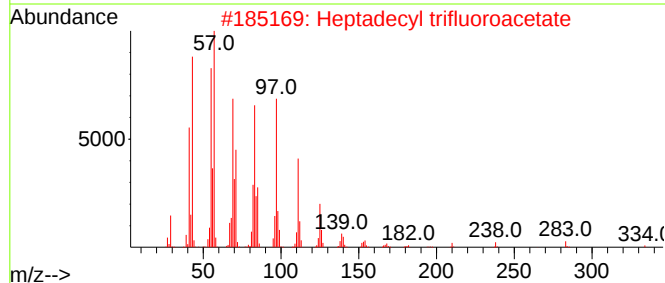
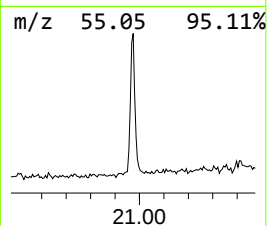
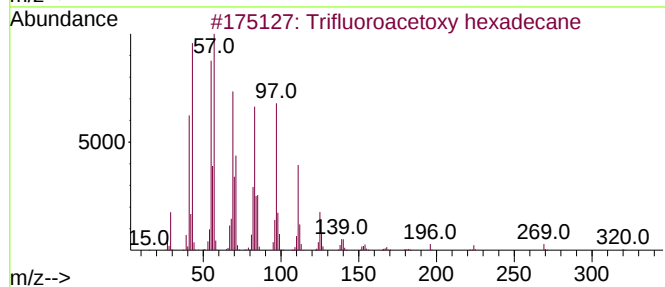
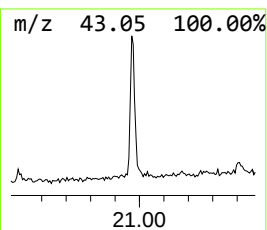
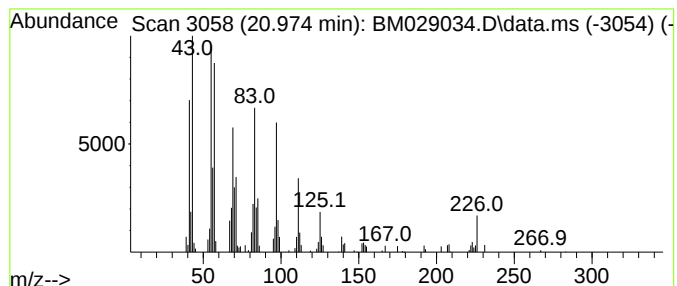
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	8.51 ng	93909	Chrysene-d12	21.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3			1-Docosene	308	C22H44	001599-67-3	93
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029034.D
Acq On : 09 Mar 2021 00:22
Operator : CG/JU
Sample : M1589-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-B

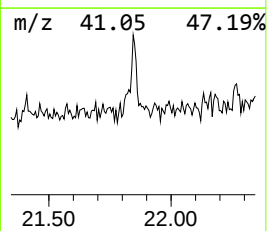
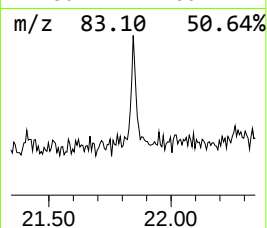
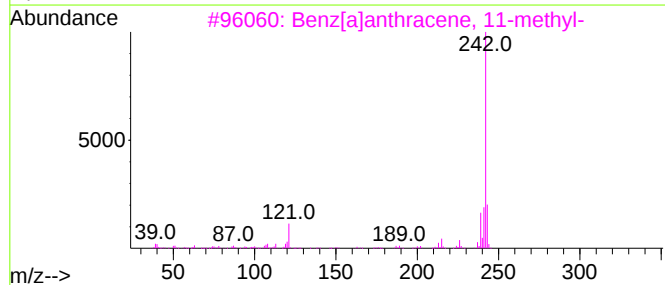
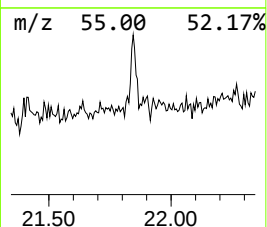
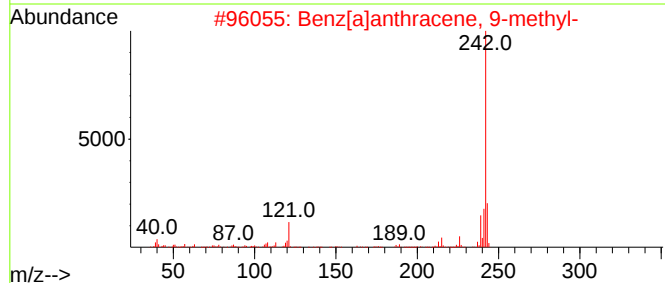
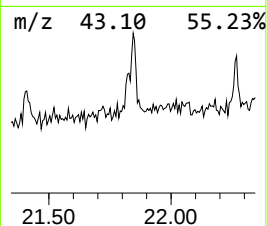
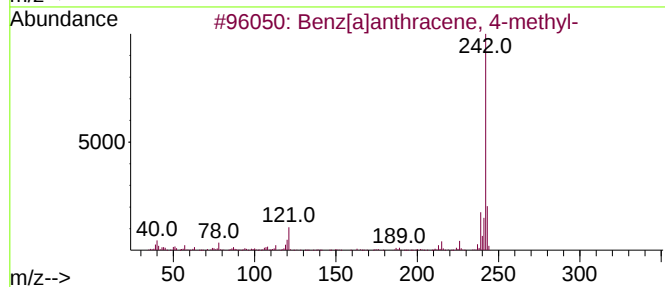
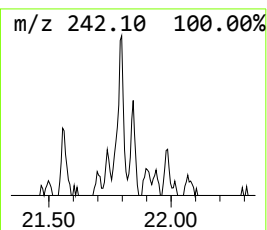
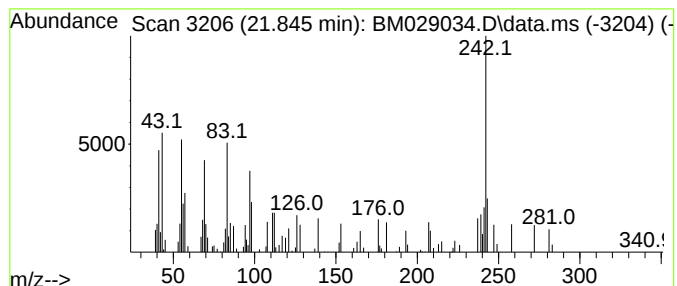
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benz[a]anthracene, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.845	2.23 ng	24565	Chrysene-d12	21.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[a]anthracene, 4-methyl-	242	C19H14	000316-49-4	60
2			Benz[a]anthracene, 9-methyl-	242	C19H14	002381-16-0	60
3			Benz[a]anthracene, 11-methyl-	242	C19H14	006111-78-0	60
4			Benz[a]anthracene, 10-methyl-	242	C19H14	002381-15-9	60
5			Chrysene, 3-methyl-	242	C19H14	003351-31-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029034.D
Acq On : 09 Mar 2021 00:22
Operator : CG/JU
Sample : M1589-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-B

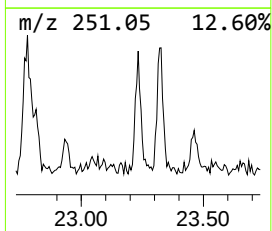
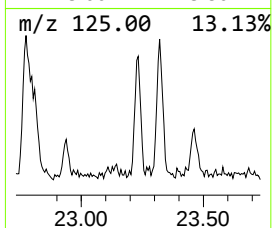
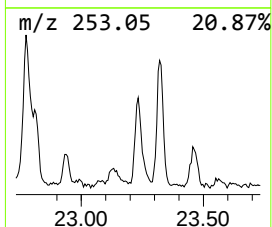
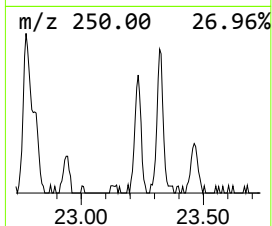
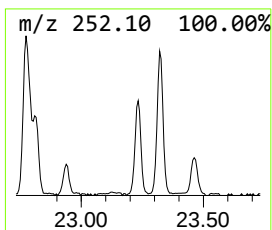
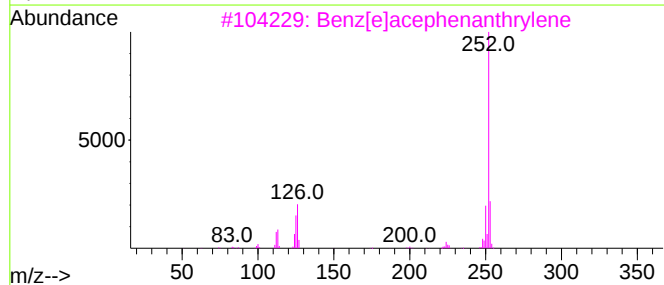
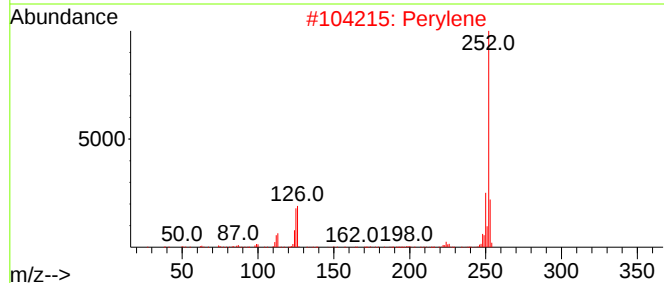
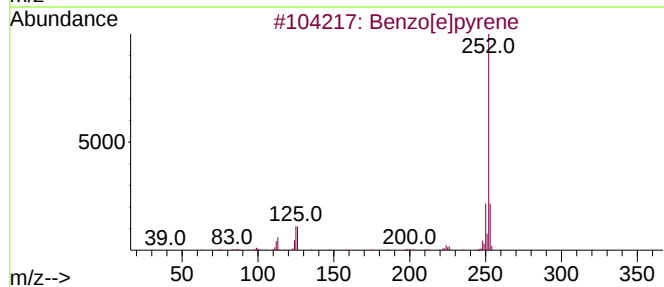
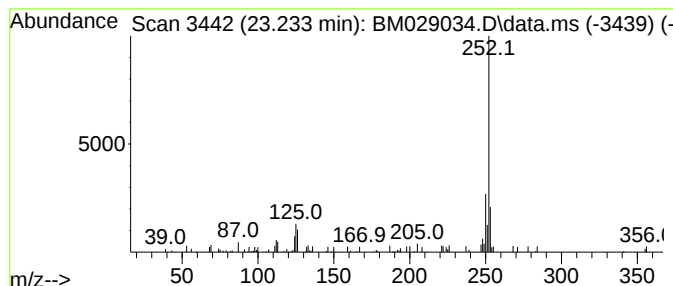
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.233	4.97 ng	33857	Perylene-d12	23.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Perylene	252	C20H12	000198-55-0	94
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90
4			Benzo[a]pyrene	252	C20H12	000050-32-8	76
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030821\
Data File : BM029034.D
Acq On : 09 Mar 2021 00:22
Operator : CG/JU
Sample : M1589-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FK-GF-02-067-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.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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n-Hexadecanoic ...	17.980	8.2	ng	45507	4	17.086	111422	20.0
4H-Cyclopenta[d]...	18.151	2.4	ng	13280	4	17.086	111422	20.0
11H-Benzo[b]flu...	19.998	2.2	ng	24523	5	21.256	220776	20.0
Trifluoroacetox...	20.974	8.5	ng	93909	5	21.256	220776	20.0
Benz[a]anthrace...	21.845	2.2	ng	24565	5	21.256	220776	20.0
Benzo[e]pyrene	23.233	5.0	ng	33857	6	23.415	136166	20.0