

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
 Data File : BF124988.D
 Acq On : 7 Aug 2021 22:50
 Operator : JU/CG
 Sample : M3293-01 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 289

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_F\METHODS\8270-BF080421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124988.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.439	567	570	574	rBV	65411	59222	3.06%	0.799%
2	6.457	740	743	746	rBV	78600	61018	3.15%	0.823%
3	6.828	803	806	809	rBB	51060	37435	1.93%	0.505%
4	7.392	898	902	904	rBB	50111	39485	2.04%	0.532%
5	8.110	1021	1024	1026	rBV	61278	52372	2.71%	0.706%
6	8.133	1026	1028	1031	rVB	30464	20655	1.07%	0.279%
7	9.186	1201	1207	1210	rBV	105322	84954	4.39%	1.146%
8	9.527	1262	1265	1267	rVV3	19347	22850	1.18%	0.308%
9	9.563	1267	1271	1274	rVV3	41874	57990	3.00%	0.782%
10	9.592	1274	1276	1279	rVB2	35784	26432	1.37%	0.356%
11	9.733	1297	1300	1303	rBV4	28000	35785	1.85%	0.483%
12	9.780	1305	1308	1311	rVB3	34850	34457	1.78%	0.465%
13	9.880	1317	1325	1328	rBV	1127730	1934751	100.00%	26.091%
14	9.910	1328	1330	1334	rVV	82362	95261	4.92%	1.285%
15	9.945	1334	1336	1339	rVB3	28682	26568	1.37%	0.358%
16	9.986	1340	1343	1348	rVB3	26586	35001	1.81%	0.472%
17	10.074	1350	1358	1364	rBV2	986423	1442362	74.55%	19.451%
18	10.151	1364	1371	1374	rBV	876155	1179313	60.95%	15.903%
19	10.204	1377	1380	1382	rBV2	45520	49855	2.58%	0.672%
20	10.286	1391	1394	1399	rBV4	60193	84347	4.36%	1.137%
21	10.427	1415	1418	1425	rBV	76430	89565	4.63%	1.208%
22	10.580	1441	1444	1447	rBV4	40097	48730	2.52%	0.657%
23	10.663	1456	1458	1461	rBV2	60108	53730	2.78%	0.725%
24	10.792	1477	1480	1483	rBV2	127051	136467	7.05%	1.840%
25	11.057	1523	1525	1528	rVB2	62982	52882	2.73%	0.713%
26	11.263	1557	1560	1566	rVB	201454	221170	11.43%	2.983%
27	11.404	1580	1584	1586	rVB	305051	280449	14.50%	3.782%
28	11.451	1589	1592	1594	rVB	79767	61549	3.18%	0.830%
29	12.304	1735	1737	1742	rVB3	73410	69112	3.57%	0.932%
30	12.598	1783	1787	1790	rVB	249782	249275	12.88%	3.362%
31	12.827	1823	1826	1831	rVB	197424	215104	11.12%	2.901%
32	12.933	1842	1844	1846	rBV2	49004	52306	2.70%	0.705%
33	13.998	2022	2025	2029	rBV2	98190	143392	7.41%	1.934%
34	14.033	2029	2031	2038	rVB	100899	95382	4.93%	1.286%
35	14.480	2101	2107	2109	rVB5	16312	19589	1.01%	0.264%
36	15.033	2196	2201	2204	rBV	54067	80795	4.18%	1.090%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.333	2248	2252	2256	rVB	28155	34210	1.77%	0.461%
38	15.398	2259	2263	2267	rVB	42398	49709	2.57%	0.670%
39	15.456	2269	2273	2276	rBV	26115	28920	1.49%	0.390%
40	16.915	2512	2521	2526	rVB2	16554	31106	1.61%	0.419%
41	17.356	2590	2596	2603	rVB	11707	21965	1.14%	0.296%

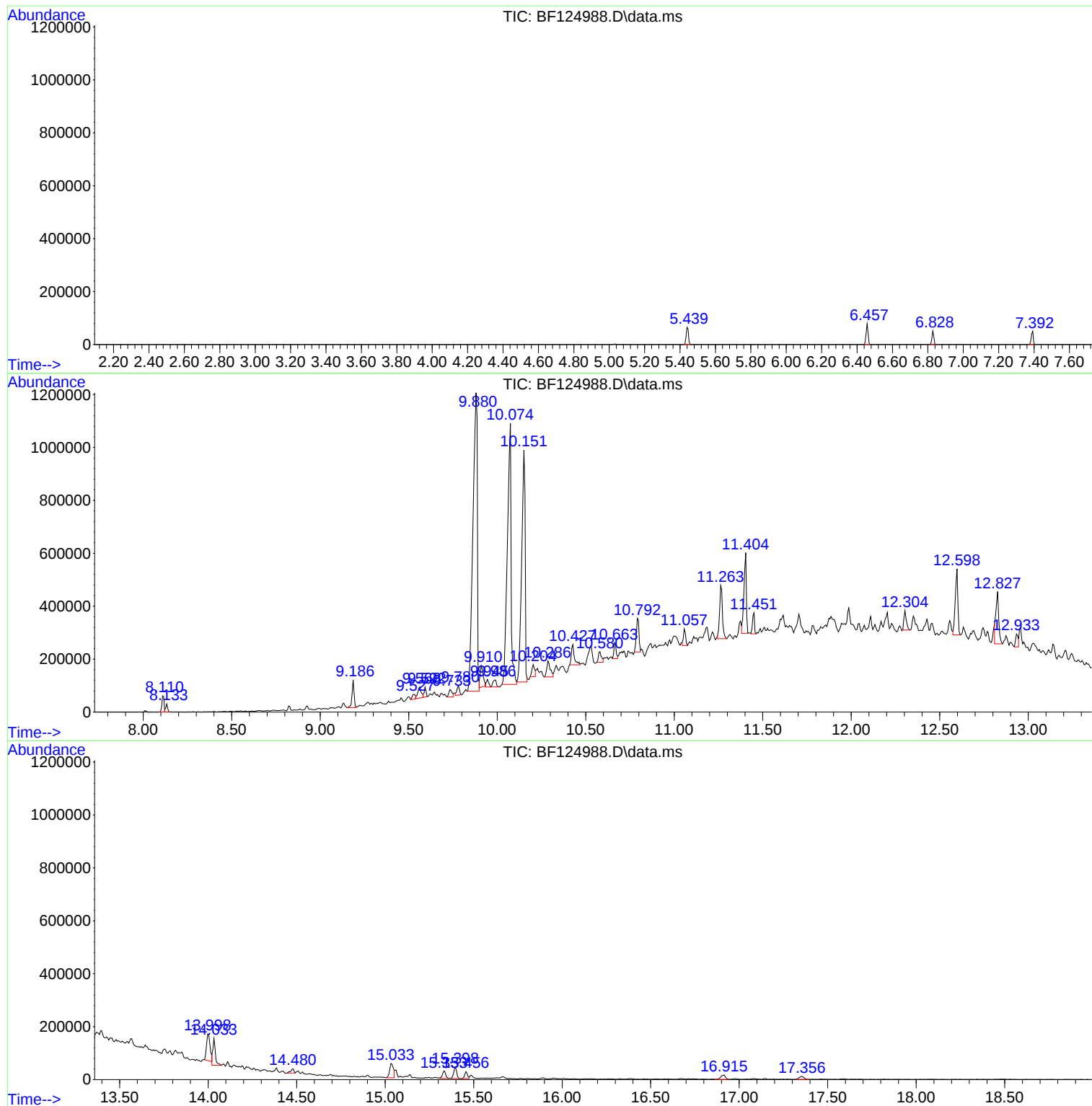
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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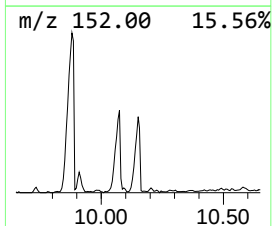
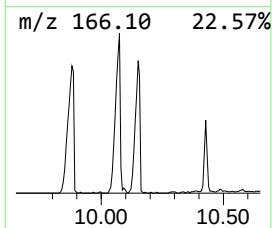
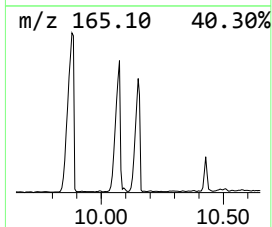
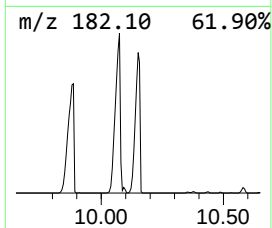
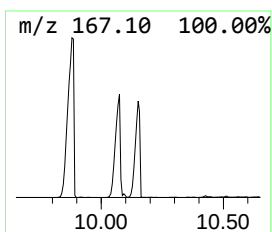
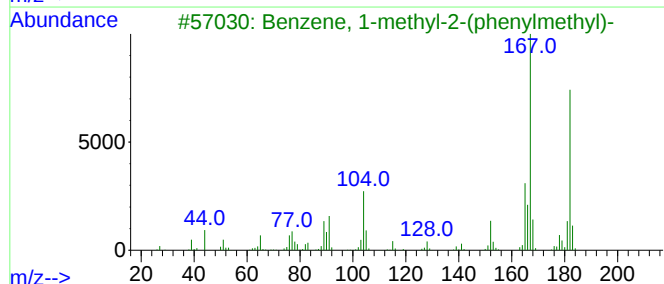
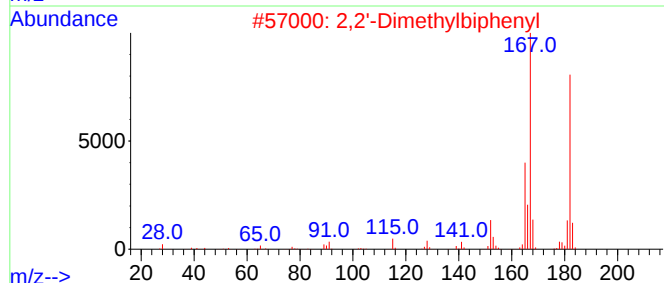
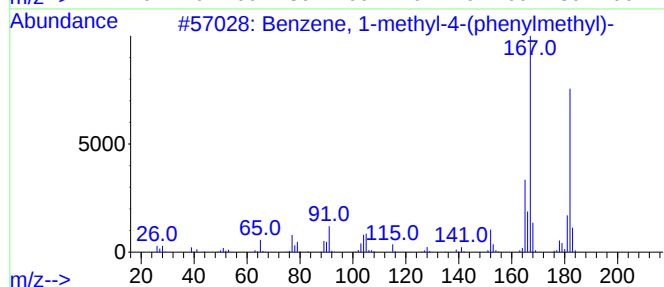
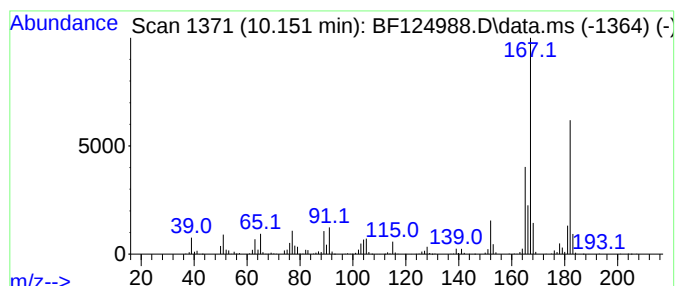
Instrument :
BNA_F
ClientSampled :
289

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzene, 1-methyl-4-(phenyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.151	12.19 ng	1179310	Acenaphthene-d10	9.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(phenylmethyl)-	182	C14H14	000620-83-7	96
2	2,2'-Dimethylbiphenyl	182	C14H14	000605-39-0	94
3	Benzene, 1-methyl-2-(phenylmethyl)-	182	C14H14	000713-36-0	93
4	1,1'-Biphenyl, 2,4'-dimethyl-	182	C14H14	000611-61-0	91
5	1H,2H,3H-Cyclopenta[a]naphthalen...	182	C14H14	001624-22-2	86



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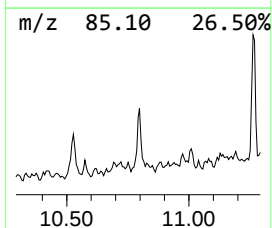
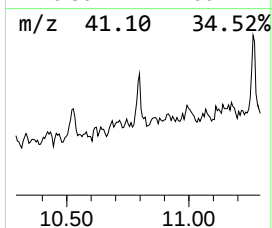
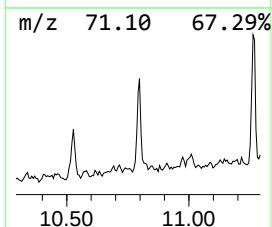
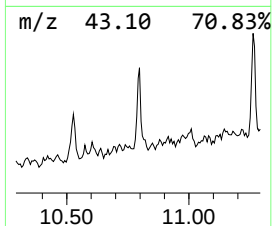
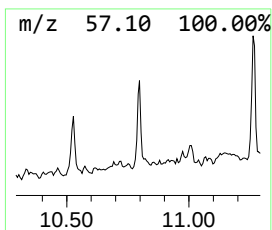
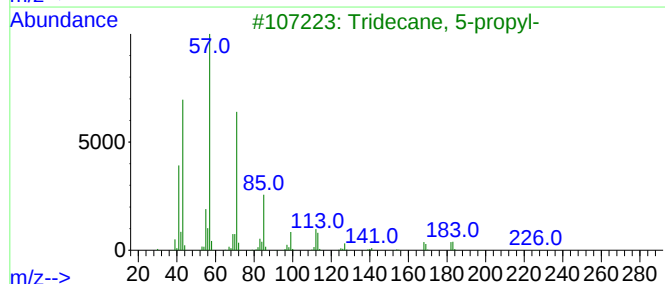
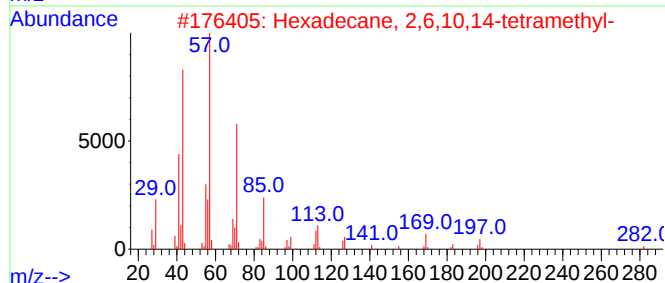
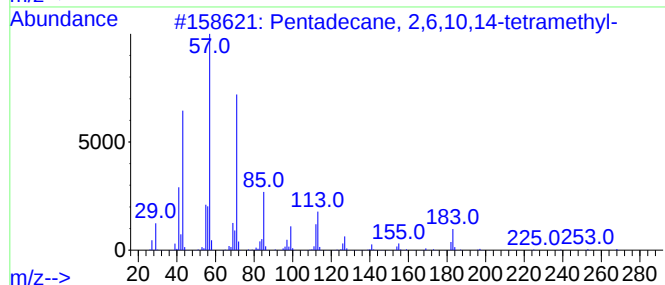
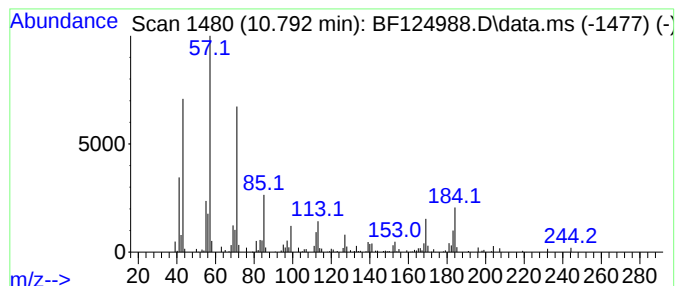
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.792	9.73 ng	136467	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	81
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
3			Tridecane, 5-propyl-	226	C16H34	055045-11-9	64
4			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	64
5			Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	62



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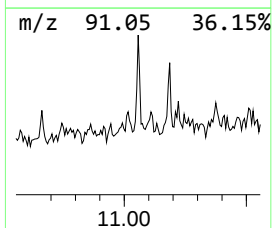
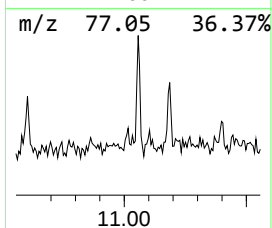
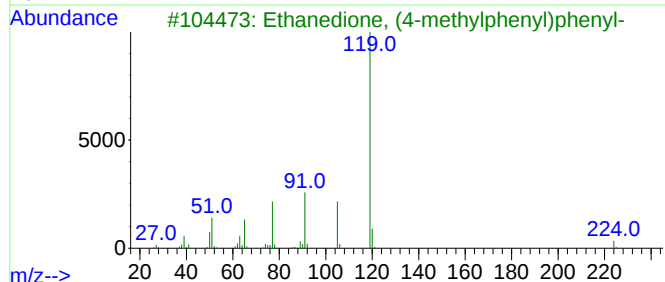
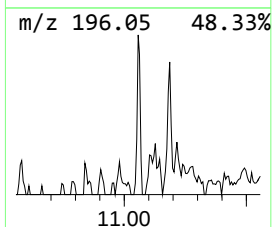
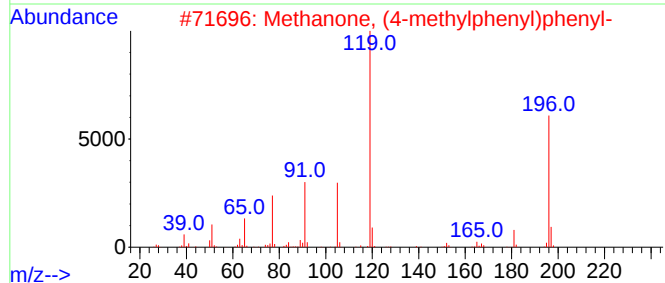
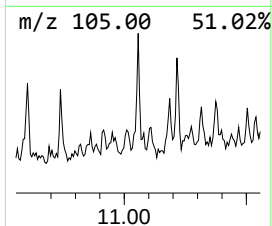
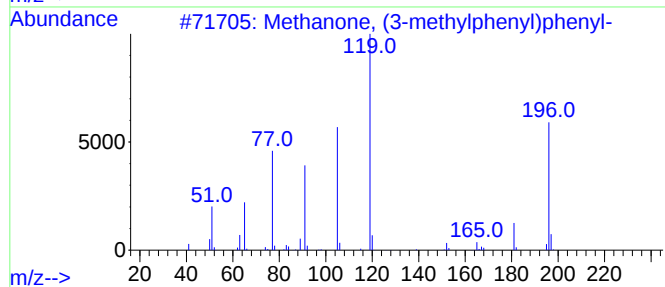
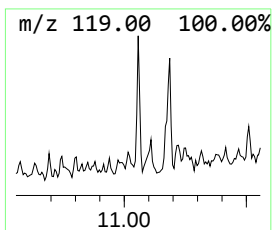
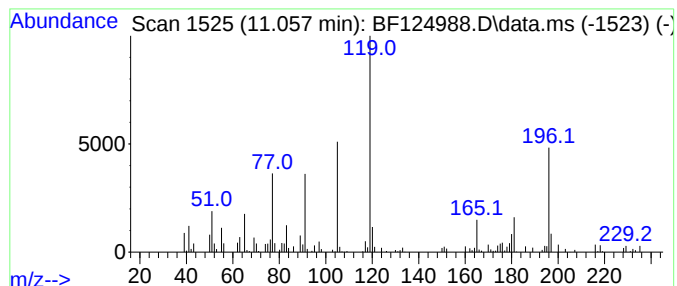
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Methanone, (3-methylphenyl)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.057	3.77 ng	52882	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (3-methylphenyl)phenyl-	196	C14H12O	000643-65-2	91
2			Methanone, (4-methylphenyl)phenyl-	196	C14H12O	000134-84-9	87
3			Ethanedione, (4-methylphenyl)phe...	224	C15H12O2	002431-00-7	47
4			4-Methyl-N-(5-methyl-3-isoxazoly...	216	C12H12N2O2	109300-30-3	43
5			o-Toluic acid, 2-methylphenyl ester	226	C15H14O2	023597-23-1	38



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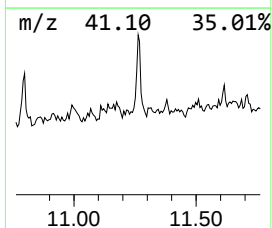
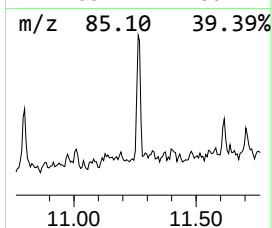
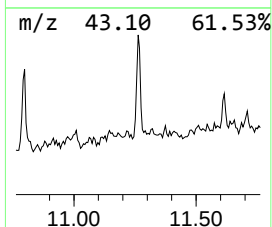
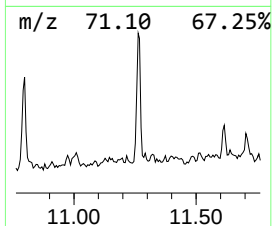
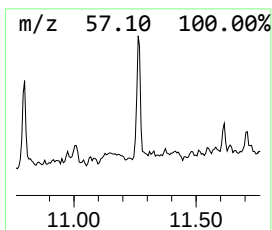
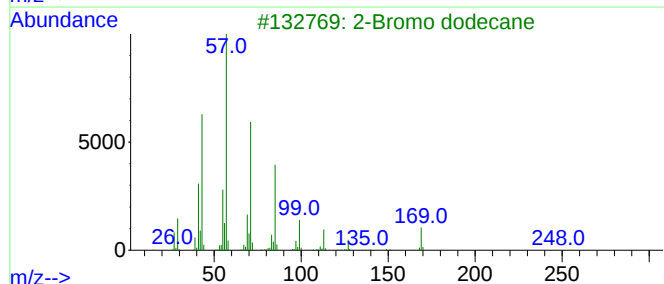
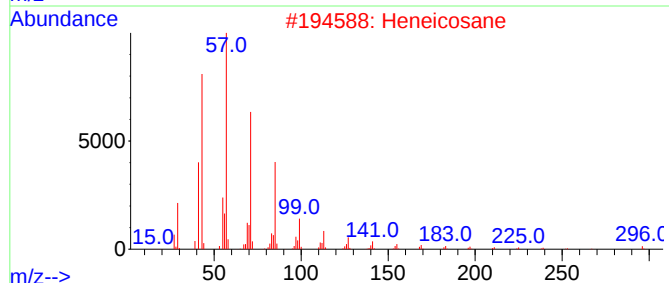
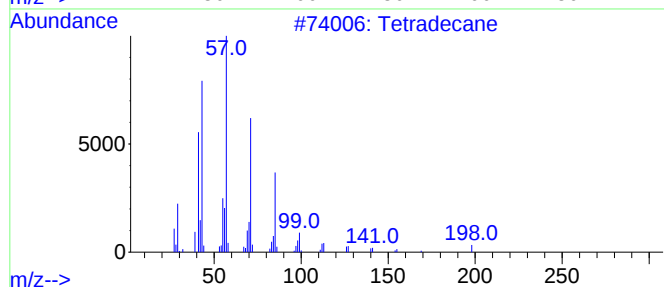
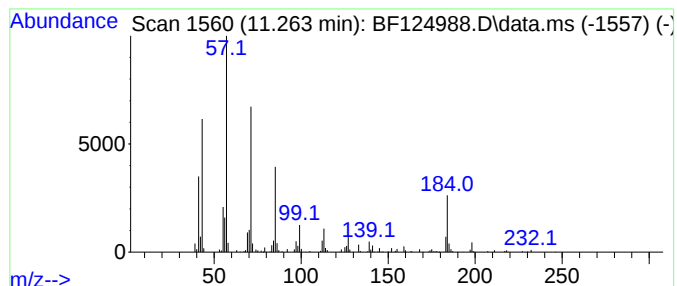
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	15.77 ng	221170	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	89
2			Heneicosane	296	C21H44	000629-94-7	76
3			2-Bromo dodecane	248	C12H25Br	013187-99-0	64
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
5			Eicosane	282	C20H42	000112-95-8	64



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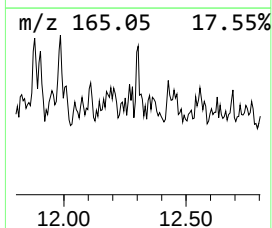
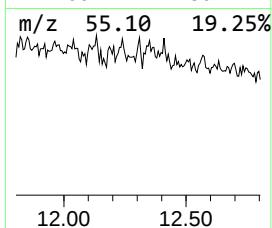
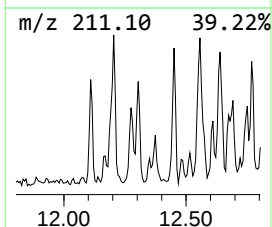
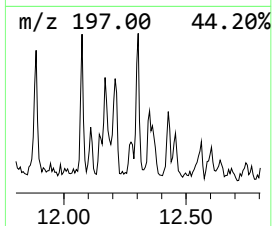
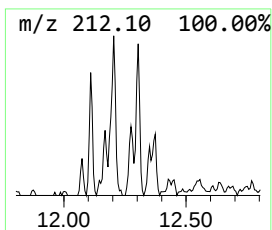
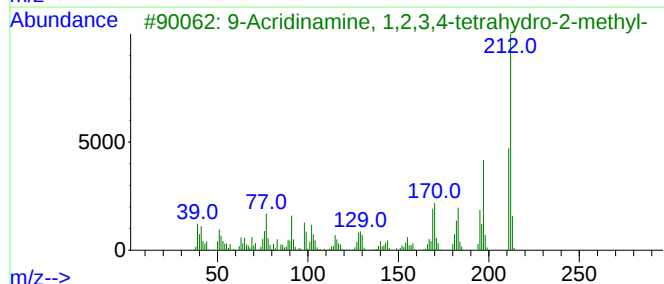
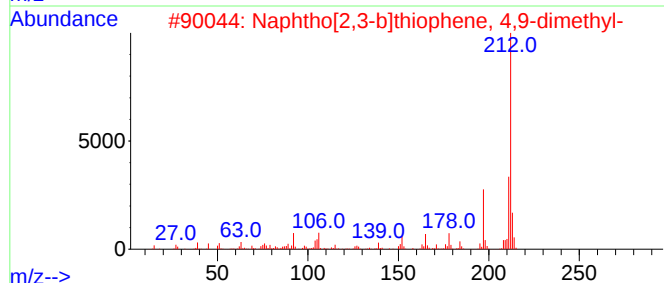
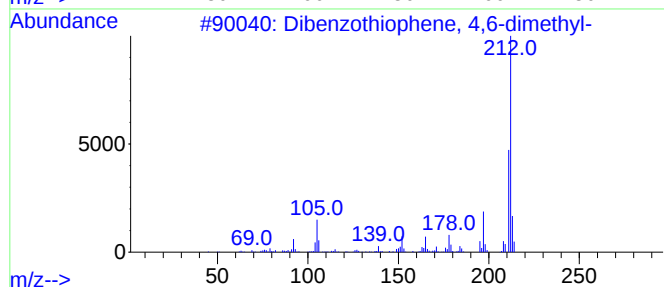
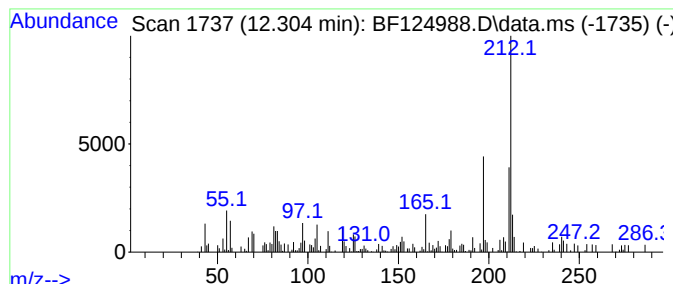
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dibenzothiophene, 4,6-dimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	4.93 ng	69112	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzothiophene, 4,6-dimethyl-	212	C14H12S	001207-12-1	86
2			Naphtho[2,3-b]thiophene, 4,9-dim...	212	C14H12S	016587-34-1	83
3			9-Acridinamine, 1,2,3,4-tetrahyd...	212	C14H16N2	1000337-15-9	80
4			2,8-Dimethyldibenzo(b,d)thiophene	212	C14H12S	001207-15-4	76
5			2,6-Dimethyldibenzothiophene	212	C14H12S	089816-75-1	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124988.D
Acq On : 7 Aug 2021 22:50
Operator : JU/CG
Sample : M3293-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

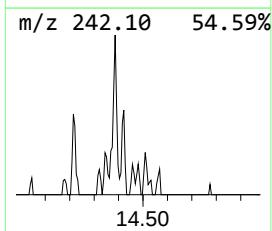
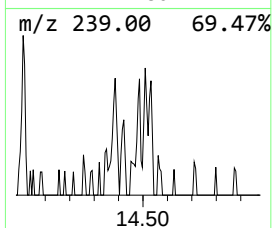
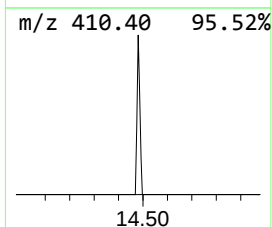
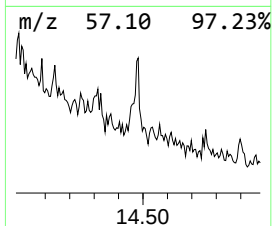
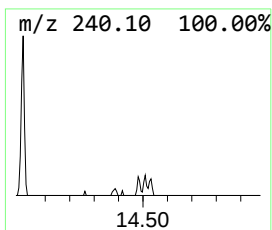
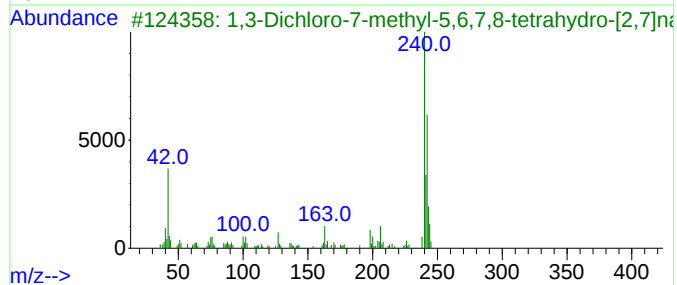
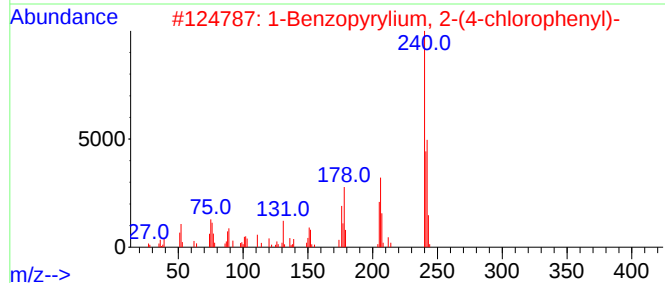
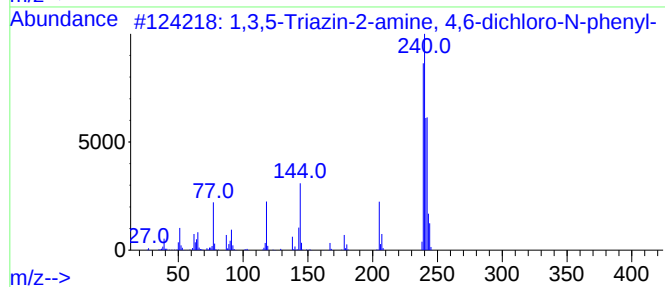
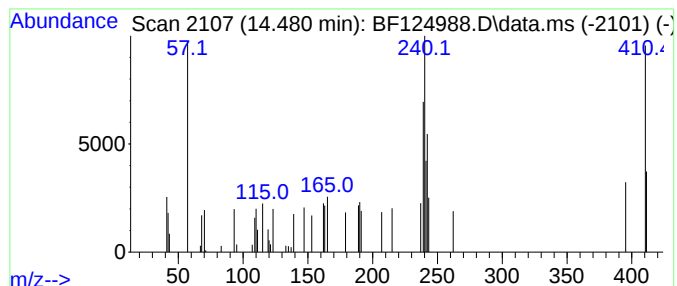
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.480 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.480	2.73 ng	19589	Chrysene-d12	14.009

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazin-2-amine, 4,6-dichl...	240	C9H6Cl2N4	002272-40-4	43	
2	1-Benzopyrylium, 2-(4-chlorophen...	241	C15H10ClO	049858-91-5	35	
3	1,3-Dichloro-7-methyl-5,6,7,8-te...	241	C10H9Cl2N3	1000274-39-1	35	
4	9-Anthraldehyde, 10-chloro-	240	C15H9ClO	010527-16-9	32	
5	5-Methyl-4-(1-naphthyl)-2-thiazo...	240	C14H12N2S	107411-05-2	22	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124988.D
Acq On : 7 Aug 2021 22:50
Operator : JU/CG
Sample : M3293-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

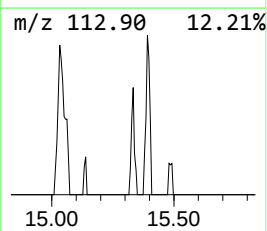
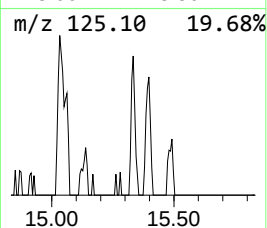
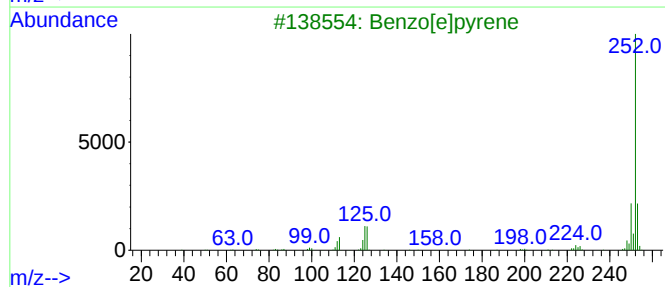
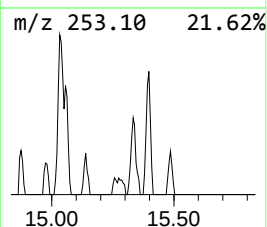
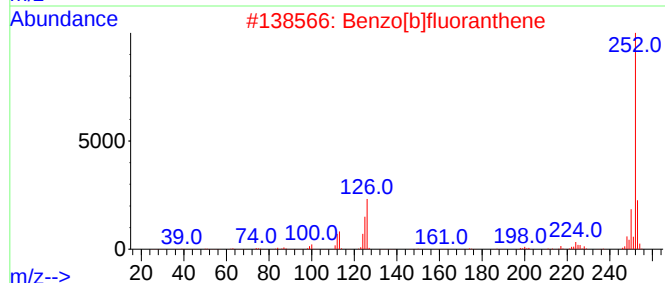
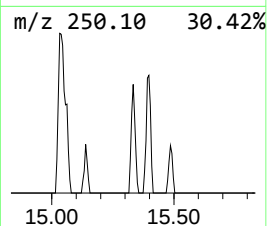
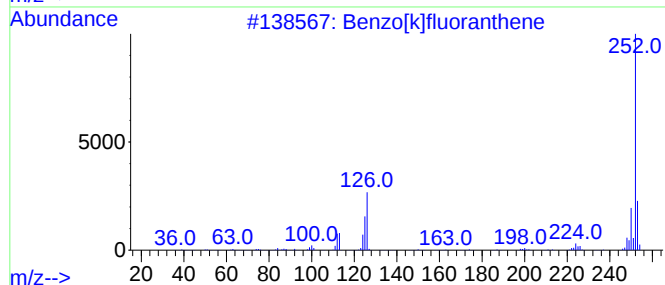
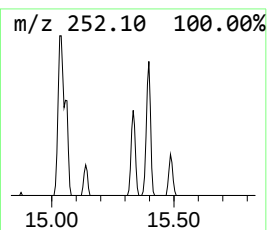
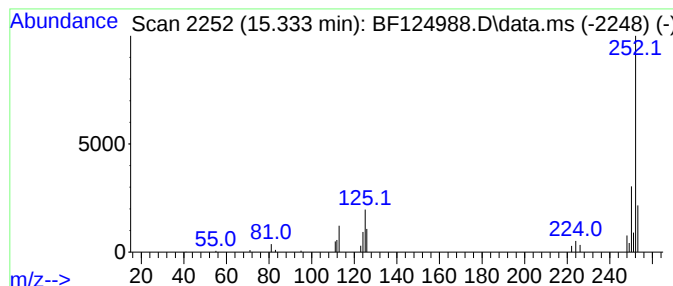
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.333	23.66 ng	34210	Perylene-d12	15.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
3			Benzo[e]pyrene	252	C20H12	000192-97-2	81
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	74
5			Benzo[a]pyrene	252	C20H12	000050-32-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124988.D
Acq On : 7 Aug 2021 22:50
Operator : JU/CG
Sample : M3293-01 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
289

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-meth...	10.151	12.2	ng	1179310	3	9.874	1934750	20.0
Pentadecane, 2,...	10.792	9.7	ng	136467	4	11.368	280449	20.0
Methanone, (3-m...	11.057	3.8	ng	52882	4	11.368	280449	20.0
Tetradecane	11.263	15.8	ng	221170	4	11.368	280449	20.0
Dibenzothiophen...	12.304	4.9	ng	69112	4	11.368	280449	20.0
unknown14.480	14.480	2.7	ng	19589	5	14.009	143392	20.0
Benzo[e]pyrene	15.333	23.7	ng	34210	6	15.456	28920	20.0