

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
 Data File : BP004130.D
 Acq On : 02 Dec 2020 15:35
 Operator : CG/JU
 Sample : L4911-02
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SK-12-1-SPB

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_P\METHODS\8270E-BP110320.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004130.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.723	83	91	98	rBV2	15836	28639	1.00%	0.117%
2	4.575	230	236	248	rBV	50321	73181	2.56%	0.298%
3	5.211	339	344	352	rBV	64229	94448	3.30%	0.385%
4	5.734	426	433	440	rBV	1339014	2076965	72.55%	8.467%
5	6.169	503	507	514	rVB	25201	41447	1.45%	0.169%
6	7.305	692	700	706	rBV	18328	32821	1.15%	0.134%
7	7.381	706	713	727	rVB	1297986	2103694	73.48%	8.576%
8	8.193	844	851	859	rBV	490768	776288	27.12%	3.165%
9	8.452	890	895	907	rBV	21856	47533	1.66%	0.194%
10	9.358	1041	1049	1059	rVB	803674	1318770	46.07%	5.376%
11	9.546	1074	1081	1092	rBV4	13769	38932	1.36%	0.159%
12	9.846	1126	1132	1139	rVB	17454	28689	1.00%	0.117%
13	11.022	1323	1332	1338	rBV	569949	969752	33.87%	3.953%
14	12.575	1590	1596	1603	rVB	27640	44136	1.54%	0.180%
15	12.751	1620	1626	1641	rBV	105101	229279	8.01%	0.935%
16	13.440	1736	1743	1752	rVB	1662651	2449958	85.58%	9.988%
17	14.251	1876	1881	1887	rBV	72533	105220	3.68%	0.429%
18	14.545	1926	1931	1936	rVB	46238	60879	2.13%	0.248%
19	14.822	1968	1978	1986	rBV	757411	1115027	38.95%	4.546%
20	16.310	2224	2231	2238	rBV	1108641	1628709	56.89%	6.640%
21	17.557	2437	2443	2448	rBV	865065	1210305	42.28%	4.934%
22	17.598	2448	2450	2457	rVV	55836	73888	2.58%	0.301%
23	17.687	2461	2465	2470	rVB	64943	89409	3.12%	0.364%
24	17.945	2505	2509	2514	rVB	28276	38263	1.34%	0.156%
25	18.222	2552	2556	2562	rVB	77548	100278	3.50%	0.409%
26	18.457	2592	2596	2603	rVB2	28144	41897	1.46%	0.171%
27	18.598	2615	2620	2624	rBV4	26569	53750	1.88%	0.219%
28	18.922	2671	2675	2681	rBV	29107	42715	1.49%	0.174%
29	19.298	2733	2739	2742	rBV4	34248	81810	2.86%	0.334%
30	19.422	2757	2760	2766	rVB2	43203	64439	2.25%	0.263%
31	19.539	2775	2780	2785	rVB	323941	404730	14.14%	1.650%
32	19.857	2831	2834	2836	rBV2	51178	62186	2.17%	0.254%
33	19.892	2836	2840	2847	rVB	336314	447888	15.64%	1.826%
34	20.063	2864	2869	2874	rBV	2454587	2862844	100.00%	11.671%
35	20.122	2876	2879	2886	rVB	32321	42230	1.48%	0.172%
36	20.657	2967	2970	2973	rBV2	42328	53685	1.88%	0.219%

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Instrument :
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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	21.086	3040	3043	3048	rBV	71339	87543	3.06%	0.357%
38	21.251	3068	3071	3075	rBV2	206105	271670	9.49%	1.108%
39	21.327	3080	3084	3088	rBV2	169898	205305	7.17%	0.837%
40	21.463	3104	3107	3116	rVB2	63902	91808	3.21%	0.374%
41	21.598	3123	3130	3134	rBV2	1124401	1822149	63.65%	7.428%
42	21.633	3134	3136	3143	rVB	230438	276159	9.65%	1.126%
43	23.298	3413	3419	3424	rBV2	307915	717974	25.08%	2.927%
44	23.821	3504	3508	3517	rVB	191059	382257	13.35%	1.558%
45	23.927	3521	3526	3536	rVB	158232	315415	11.02%	1.286%
46	24.039	3538	3545	3551	rBV	725174	1424789	49.77%	5.808%

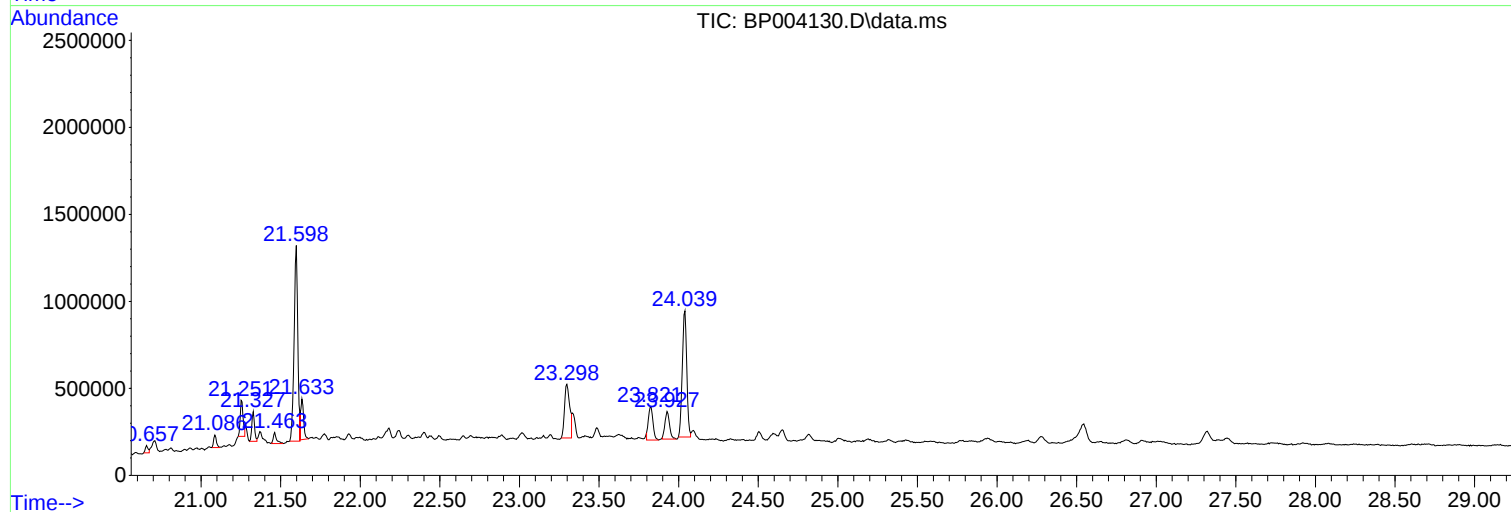
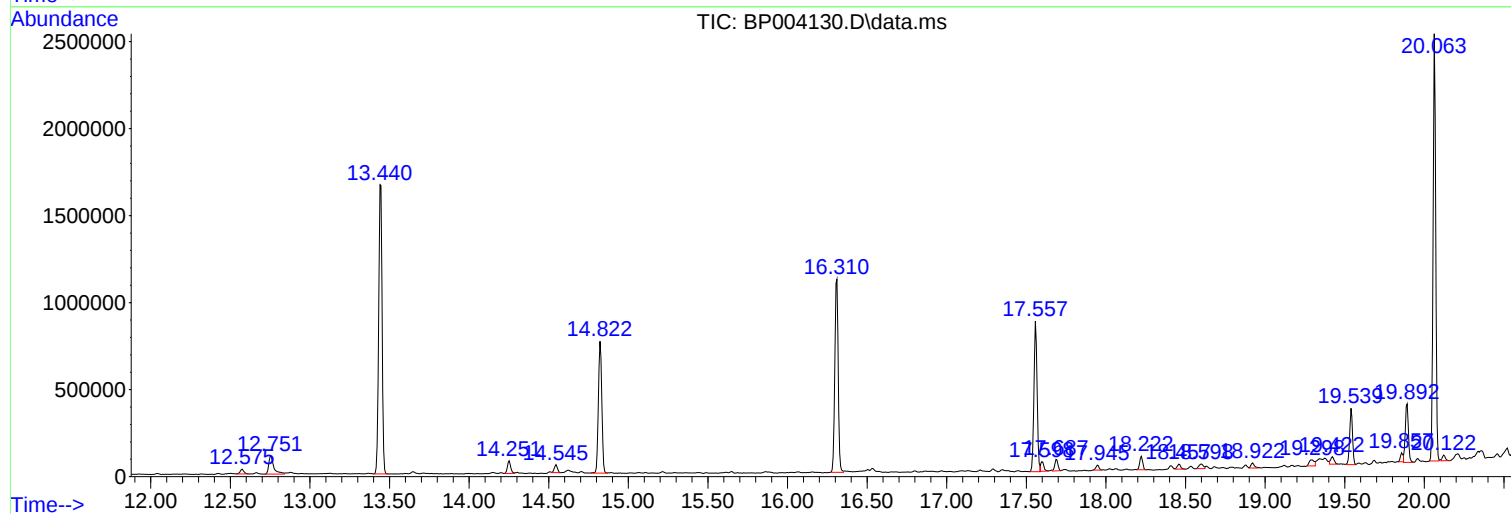
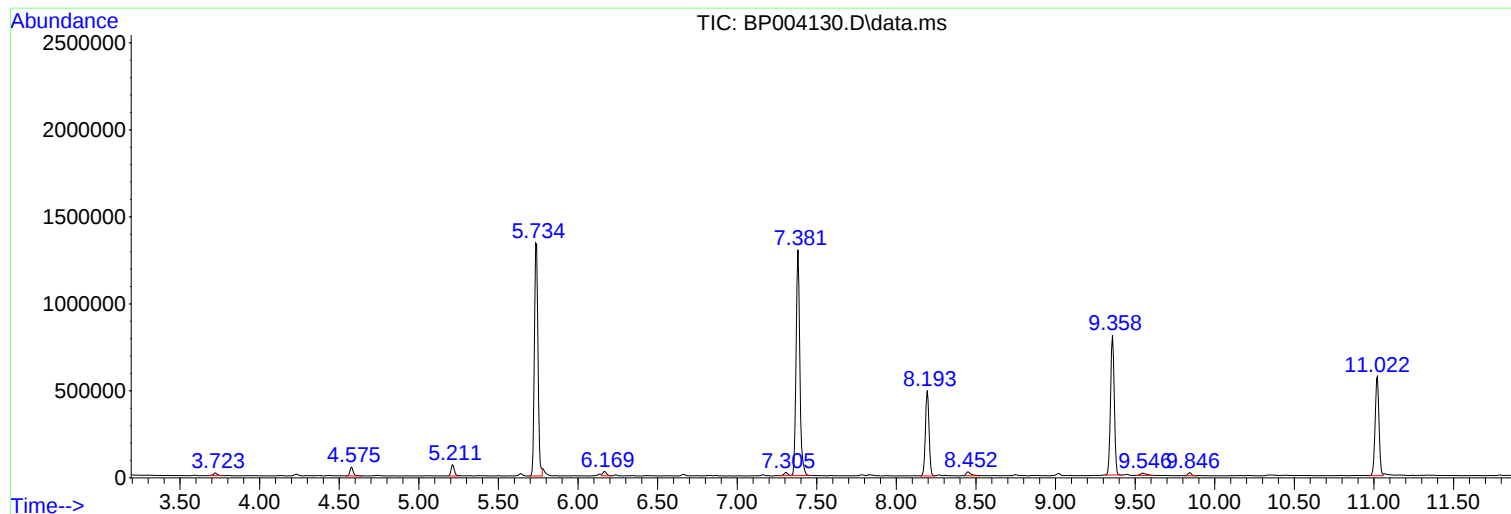
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SK-12-1-SPB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.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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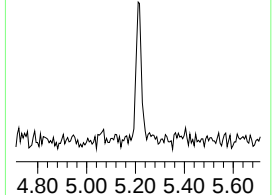
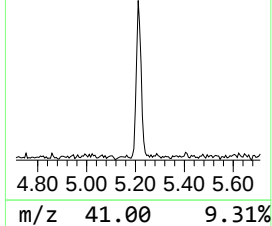
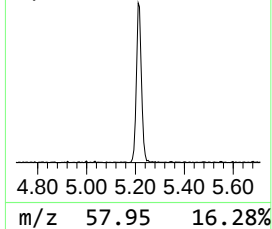
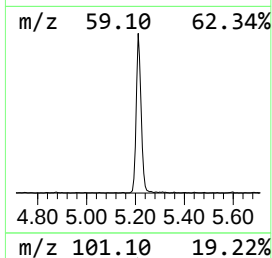
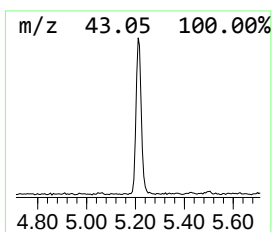
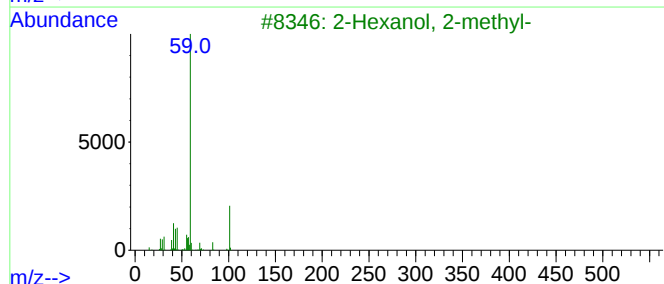
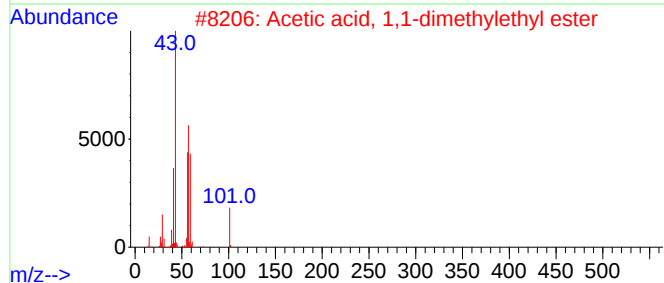
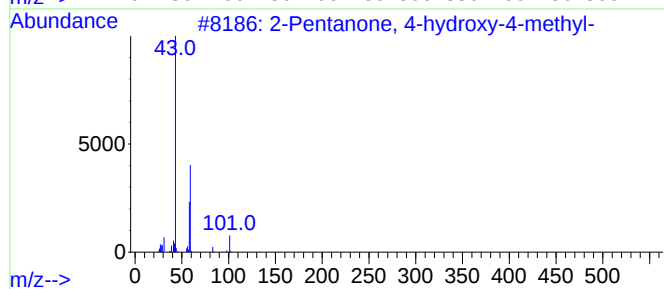
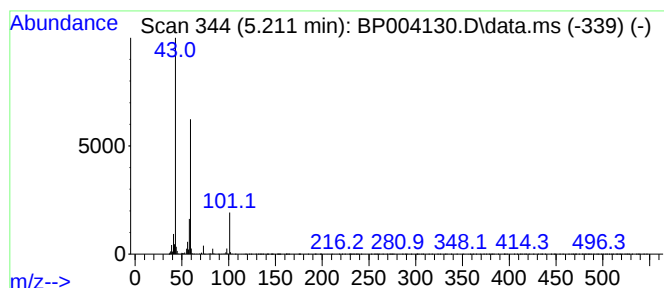
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.211	2.43 ng	94448	1,4-Dichlorobenzene-d4	8.193

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	3-Hexanol	102	C6H14O	000623-37-0	28		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25		



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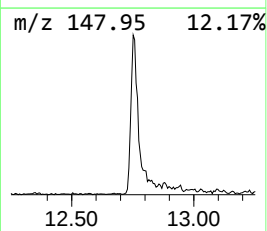
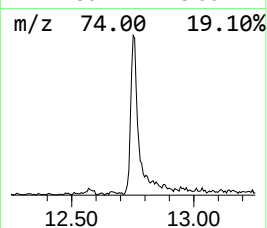
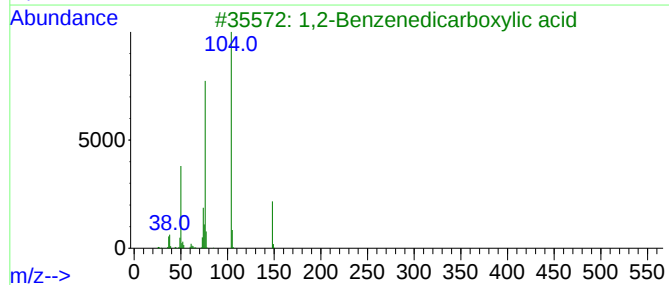
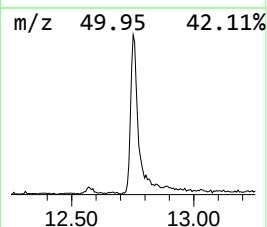
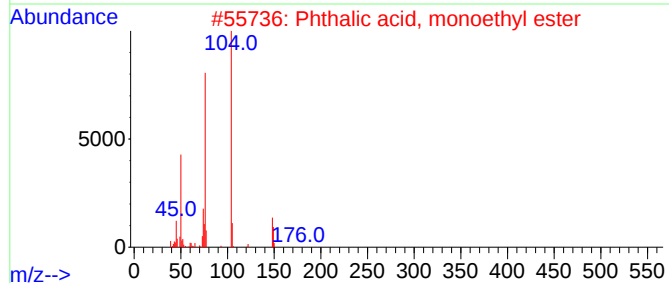
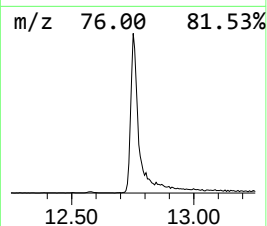
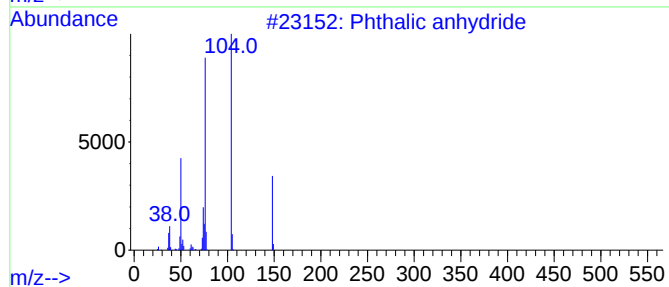
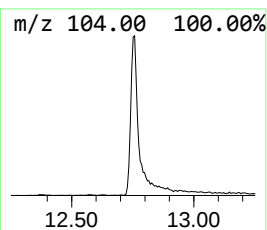
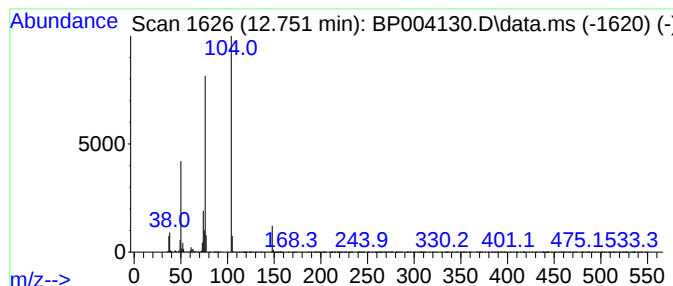
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phthalic anhydride Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.752	4.73 ng	229279	Naphthalene-d8	11.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	96
2			Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	90
3			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	90
4			Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	86
5			Phthalamic acid	165	C8H7NO3	000088-97-1	74



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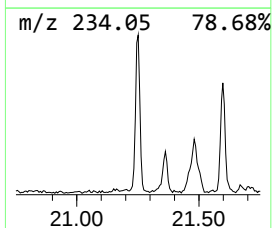
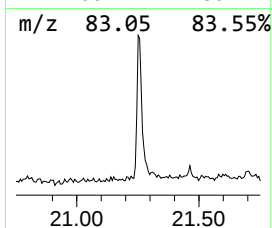
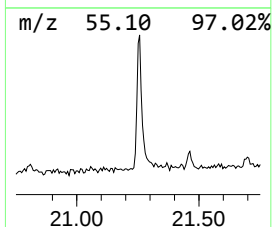
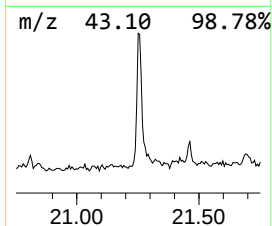
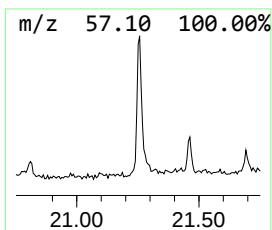
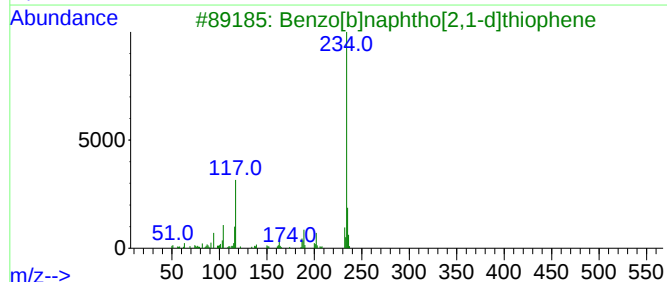
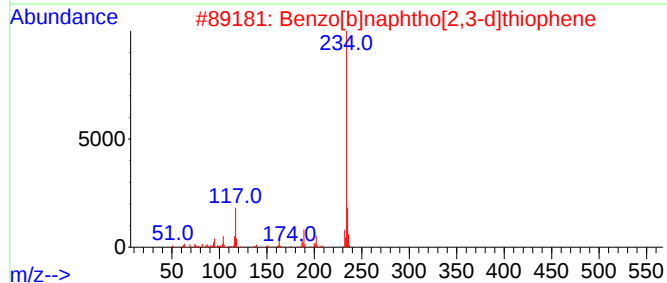
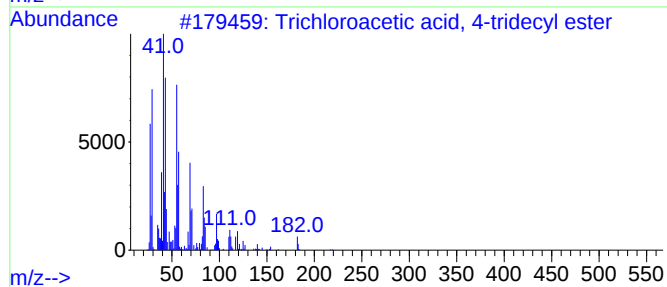
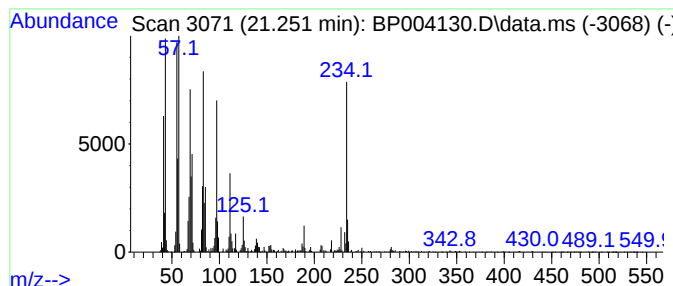
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown21.25 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	2.98 ng	271670	Chrysene-d12	21.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, 4-tridecyl...	344	C15H27Cl3O2	1000282-06-5	32
2			Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	25
3			Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	25
4			Anthra(1,2-b)thiophene	234	C16H10S	000227-86-1	25
5			Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	15



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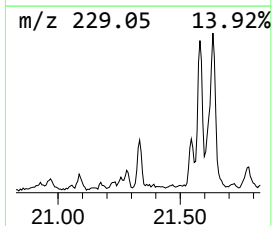
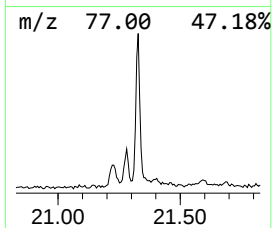
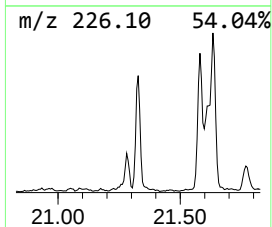
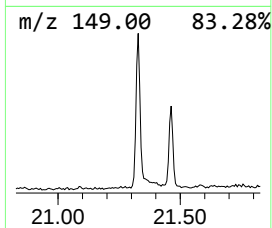
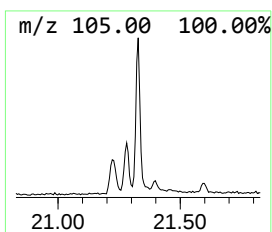
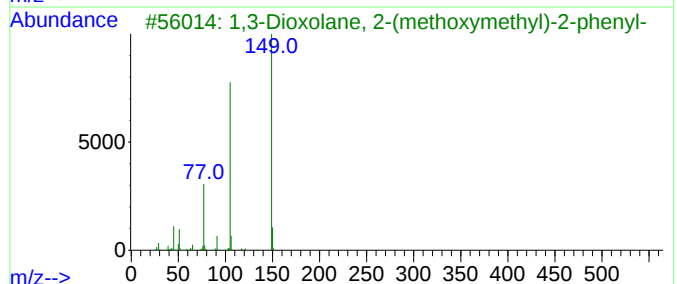
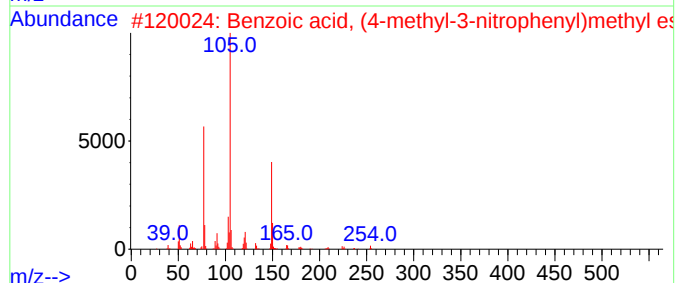
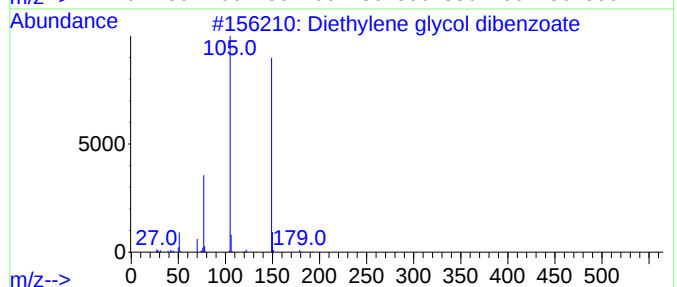
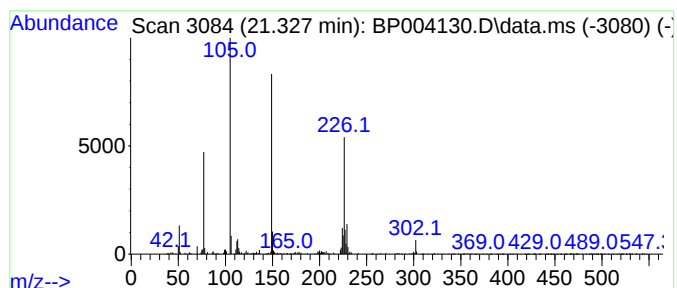
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.328	2.25 ng	205305	Chrysene-d12	21.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	52
2			Benzoic acid, (4-methyl-3-nitrop...	271	C15H13NO4	1000368-22-8	50
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	50
4			2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	43
5			2-Bromomethyl-2-phenyl[1,3]dioxo...	242	C10H11BrO2	003418-21-1	43



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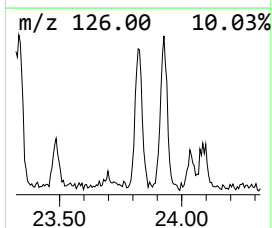
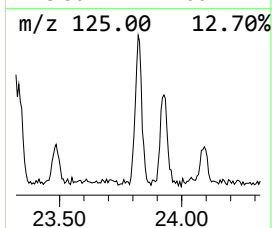
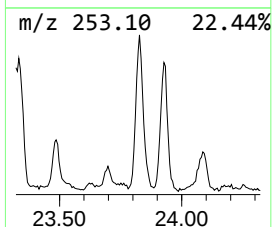
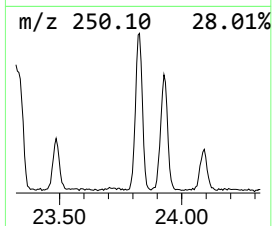
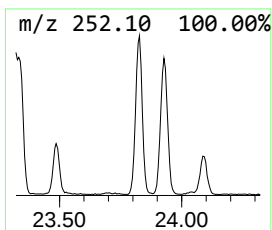
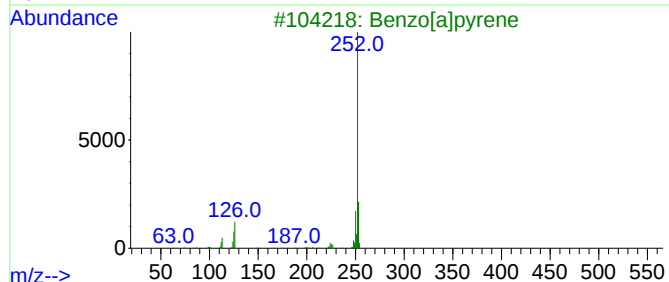
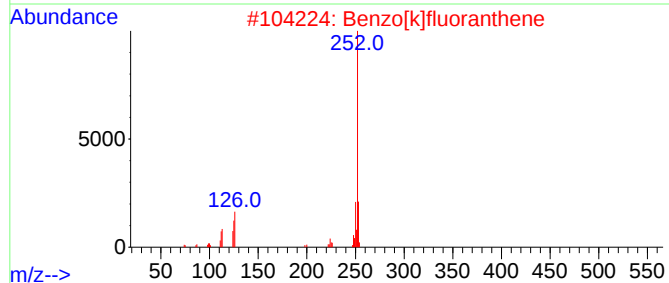
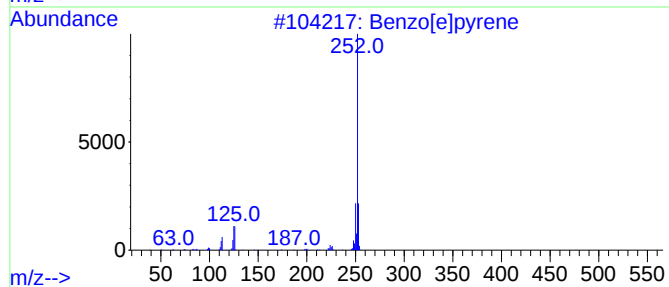
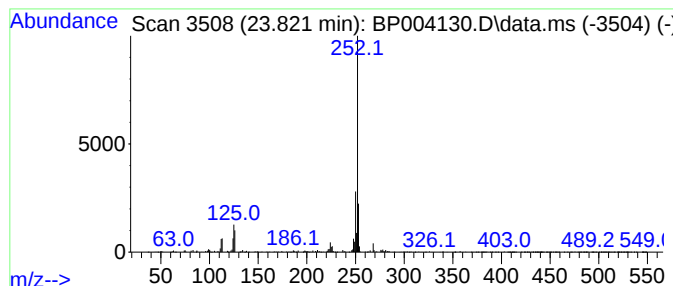
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.822	5.37 ng	382257	Perylene-d12	24.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	99
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3			Benzo[a]pyrene	252	C20H12	000050-32-8	95
4			Perylene	252	C20H12	000198-55-0	95
5			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120220\
Data File : BP004130.D
Acq On : 02 Dec 2020 15:35
Operator : CG/JU
Sample : L4911-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SK-12-1-SPB

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.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
2-Pentanone, 4-...	5.211	2.4	ng	94448	1	8.193	776288	20.0
Phthalic anhydride	12.752	4.7	ng	229279	2	11.022	969752	20.0
unknown21.25	21.251	3.0	ng	271670	5	21.598	1822150	20.0
Diethylene glyc...	21.328	2.3	ng	205305	5	21.598	1822150	20.0
Benzo[e]pyrene	23.822	5.4	ng	382257	6	24.039	1424790	20.0