

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110321\
 Data File : BP007824.D
 Acq On : 03 Nov 2021 15:56
 Operator : CG/JU
 Sample : M4427-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 FDR-BH-6-20211029-7.5-8

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-BP110221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.099	133	138	151	rBV	113991	180346	1.36%	0.257%
2	5.499	369	376	383	rVV	3646532	5434168	40.89%	7.740%
3	5.934	436	450	458	rBV3	56288	140461	1.06%	0.200%
4	7.093	639	647	663	rVB	3557585	5825779	43.83%	8.298%
5	7.916	780	787	793	rBV	787426	1220110	9.18%	1.738%
6	8.687	911	918	923	rBV	77611	149669	1.13%	0.213%
7	9.075	968	984	995	rBV	2094287	3644678	27.42%	5.191%
8	10.204	1172	1176	1182	rVB	94370	144386	1.09%	0.206%
9	10.504	1219	1227	1236	rBV	412790	666046	5.01%	0.949%
10	10.722	1255	1264	1269	rBV	1054957	1806939	13.59%	2.574%
11	10.775	1269	1273	1279	rVB	142849	250414	1.88%	0.357%
12	12.381	1539	1546	1552	rBV	92059	146958	1.11%	0.209%
13	13.181	1675	1682	1693	rBV	5443183	8256814	62.12%	11.761%
14	13.740	1764	1777	1785	rBV3	39085	134752	1.01%	0.192%
15	14.557	1908	1916	1922	rBV	1677644	2517002	18.94%	3.585%
16	15.116	2003	2011	2017	rBV2	68787	241953	1.82%	0.345%
17	15.604	2089	2094	2098	rVB3	88776	135295	1.02%	0.193%
18	16.051	2163	2170	2178	rVB	5415635	7816211	58.81%	11.133%
19	17.310	2378	2384	2389	rBV	2260062	3256191	24.50%	4.638%
20	17.351	2389	2391	2398	rVV	264546	383215	2.88%	0.546%
21	17.439	2402	2406	2412	rVB2	215018	332640	2.50%	0.474%
22	18.210	2533	2537	2545	rVB2	870256	1152421	8.67%	1.641%
23	18.363	2559	2563	2567	rBV4	80501	154186	1.16%	0.220%
24	18.498	2583	2586	2593	rVB2	108143	157742	1.19%	0.225%
25	19.069	2680	2683	2687	rBV	113235	145847	1.10%	0.208%
26	19.328	2722	2727	2731	rBV	347167	486471	3.66%	0.693%
27	19.380	2733	2736	2738	rBV2	121969	148985	1.12%	0.212%
28	19.445	2743	2747	2754	rVV2	406142	576532	4.34%	0.821%
29	19.675	2782	2786	2794	rVB	404553	616551	4.64%	0.878%
30	19.875	2815	2820	2826	rVB	10388867	13291293	100.00%	18.931%
31	20.186	2871	2873	2878	rVB	149605	138355	1.04%	0.197%
32	20.669	2952	2955	2959	rVB	159126	165412	1.24%	0.236%
33	21.116	3027	3031	3038	rVB3	691772	951617	7.16%	1.355%
34	21.404	3074	3080	3084	rBV	3345347	4517694	33.99%	6.435%
35	21.439	3084	3086	3097	rVB	274909	356623	2.68%	0.508%
36	21.563	3104	3107	3113	rBV	225259	291207	2.19%	0.415%

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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_P\Methods\8270E-BP110221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.039	3184	3188	3195	rVB3	237536	371040	2.79%	0.528%
38	23.839	3487	3494	3502	rBV2	1970748	4001393	30.11%	5.699%

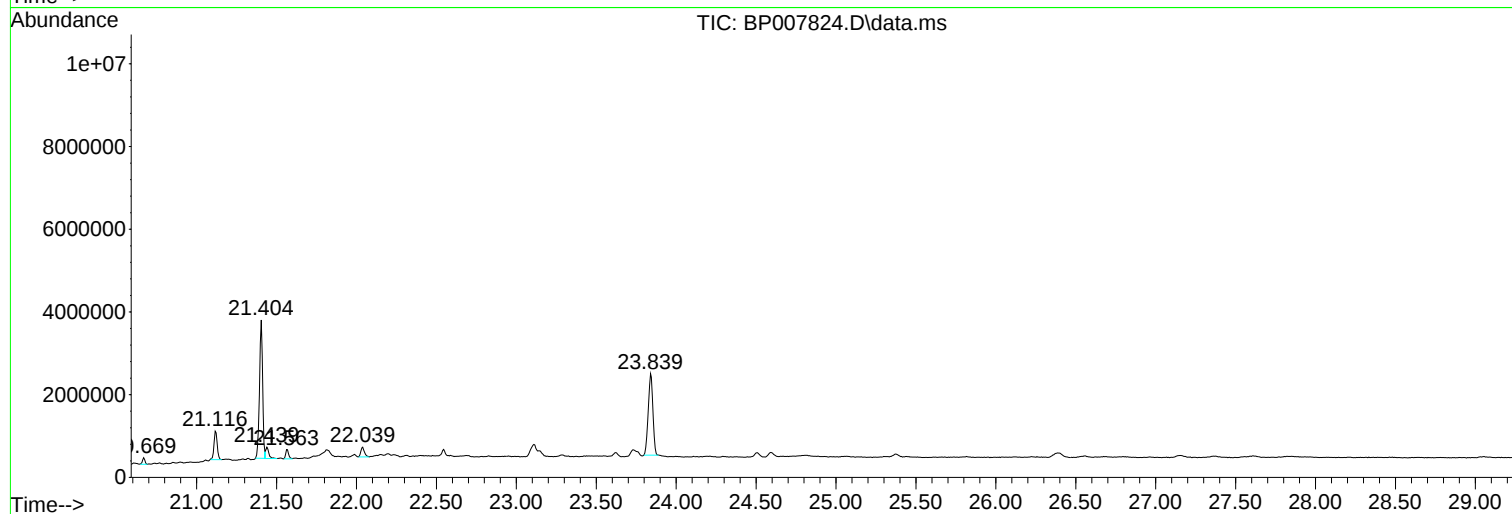
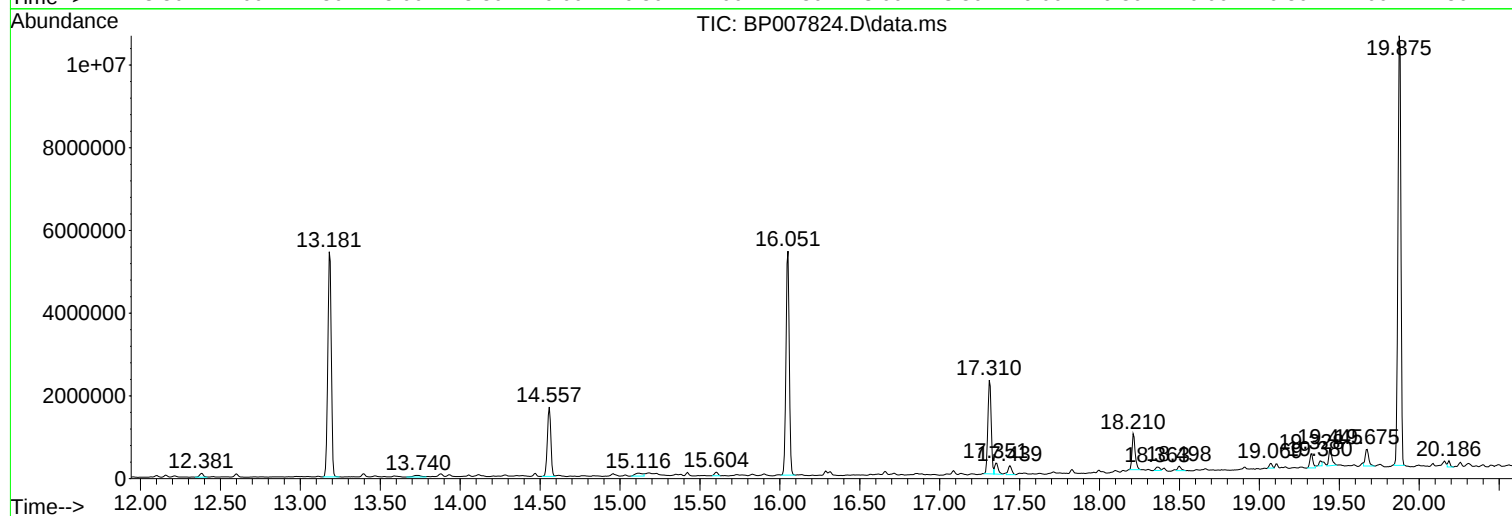
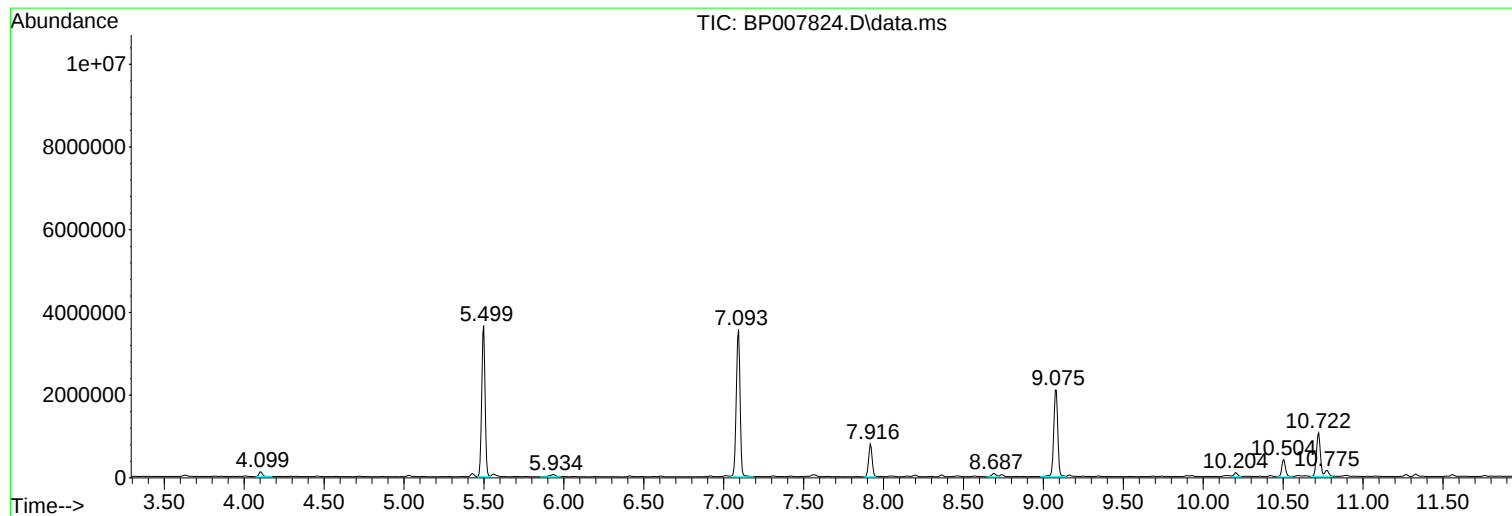
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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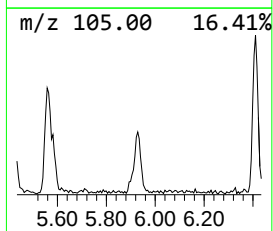
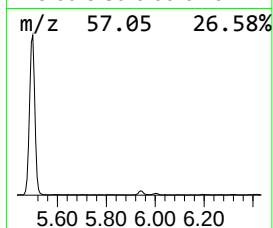
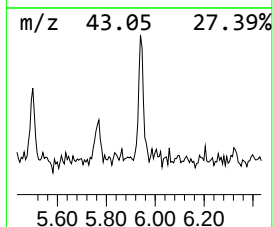
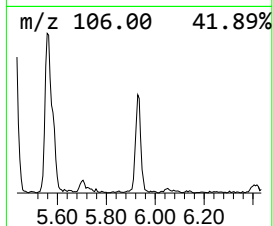
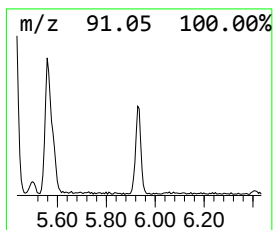
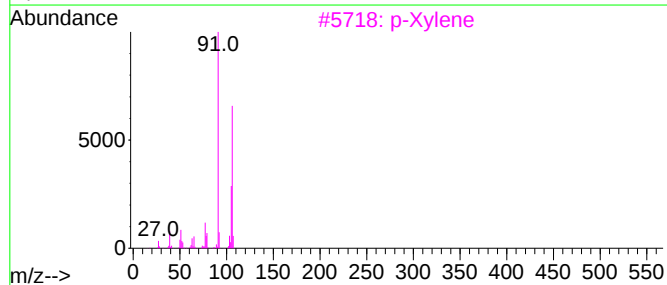
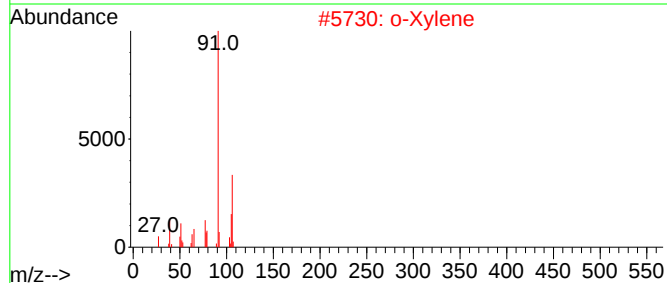
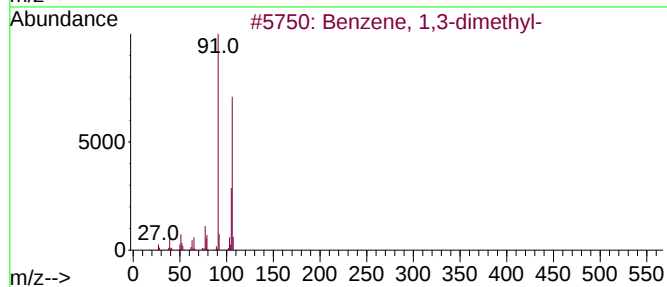
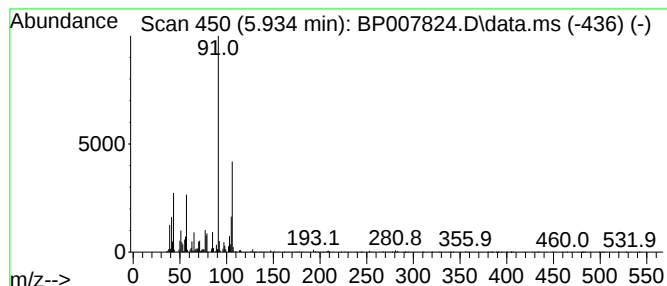
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.934	2.30 ng	140461	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	81
2			o-Xylene	106	C8H10	000095-47-6	81
3			p-Xylene	106	C8H10	000106-42-3	81
4			Ethylbenzene	106	C8H10	000100-41-4	72
5			1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	59



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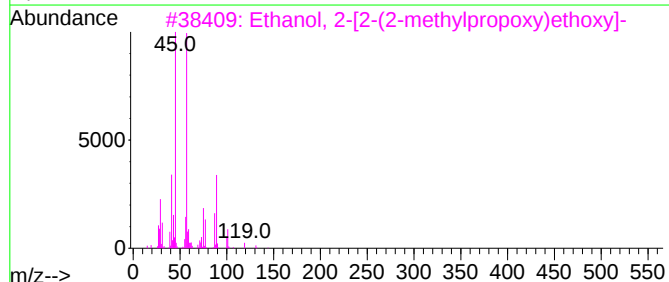
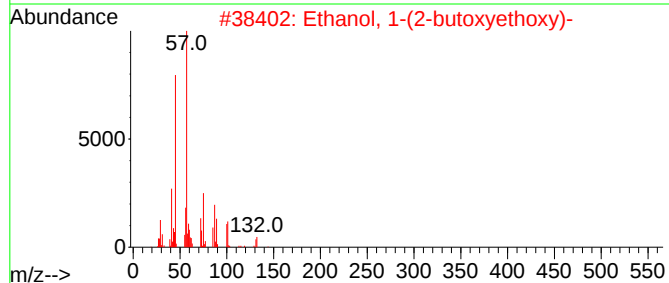
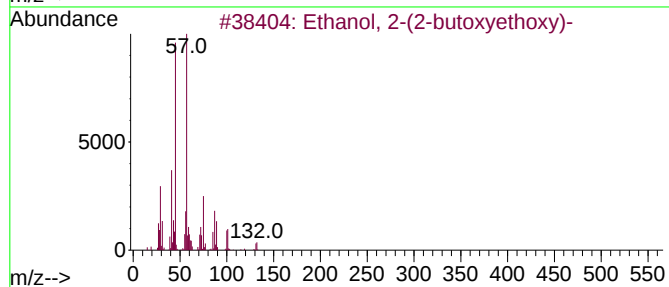
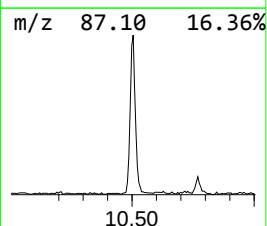
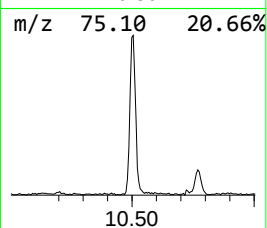
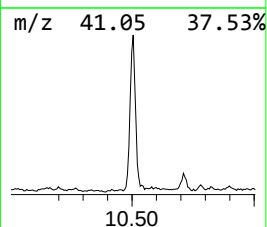
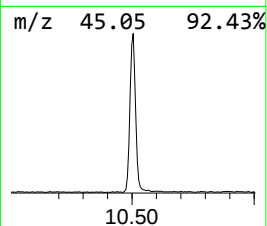
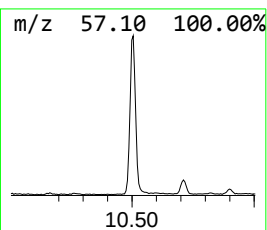
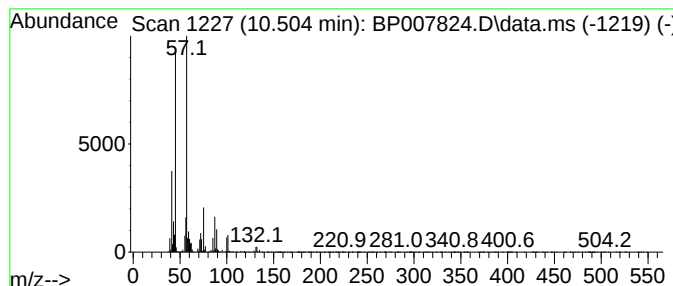
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.505	7.37 ng	666046	Naphthalene-d8	10.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	72
4			Propanoic acid, 2-hydroxy-, 2-methyl-	146	C7H14O3	000585-24-0	59
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52



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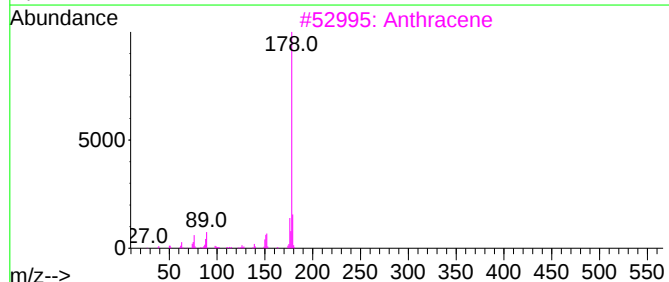
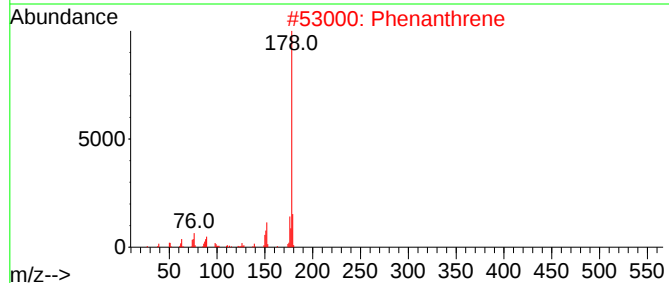
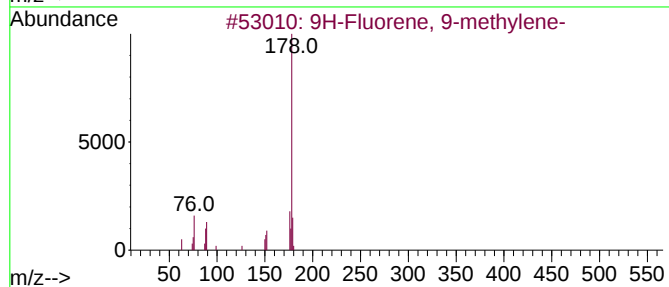
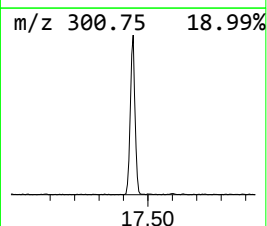
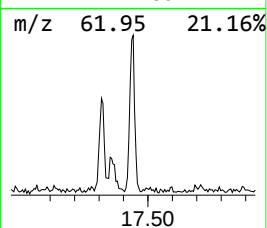
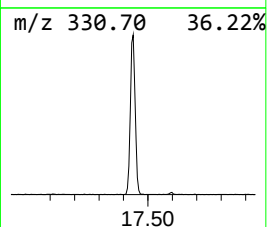
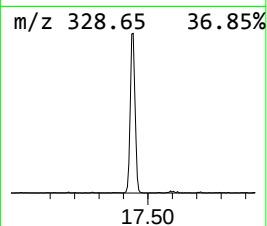
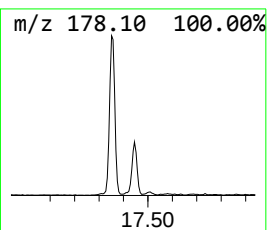
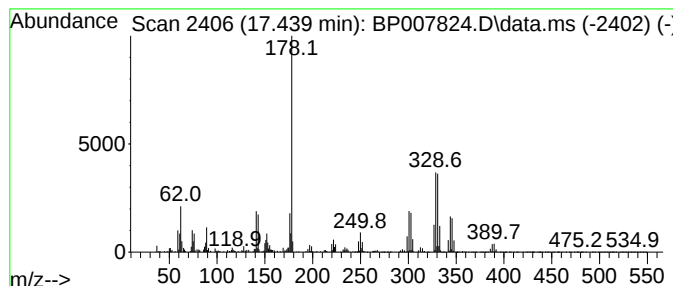
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown17.439 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.439	2.04 ng	332640	Phenanthrene-d10	17.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9H-Fluorene, 9-methylene-	178	C14H10	004425-82-5	38
2		Phenanthrene	178	C14H10	000085-01-8	35
3		Anthracene	178	C14H10	000120-12-7	20
4		Diphenylacetylene	178	C14H10	000501-65-5	20
5		1,2,4-Triazin-3-amine, 5,6-diphe...	248	C15H12N4	004511-99-3	18



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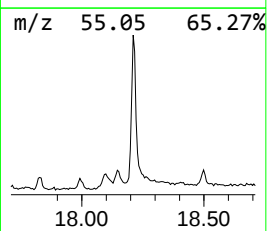
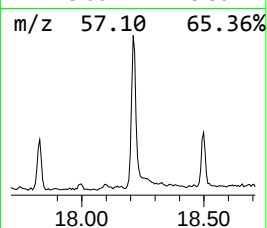
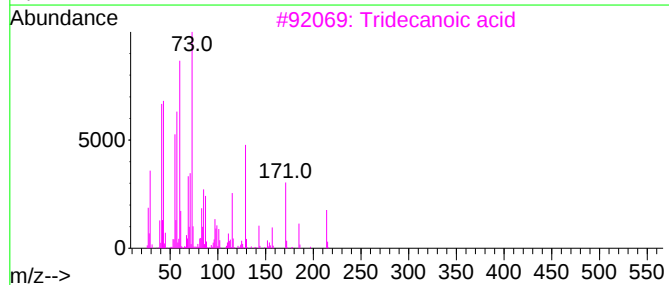
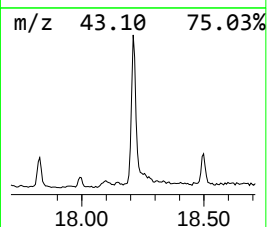
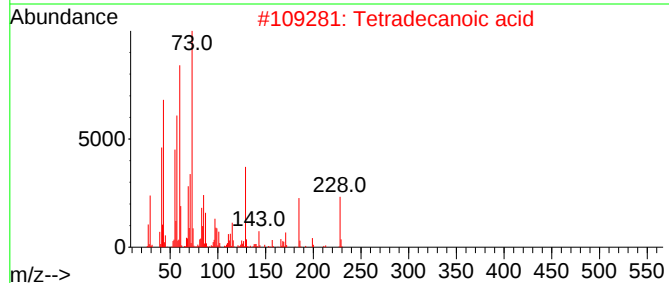
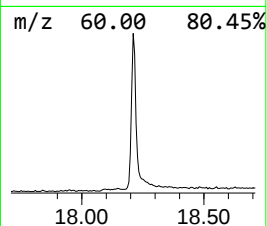
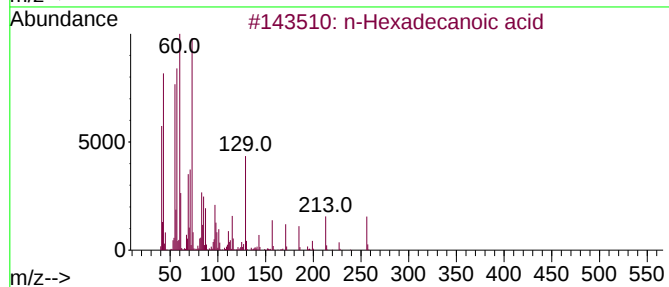
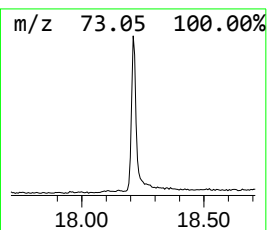
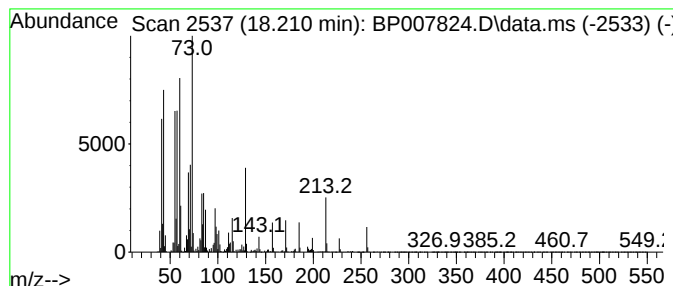
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.210	7.08 ng	1152420	Phenanthrene-d10	17.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3			Tridecanoic acid	214	C13H26O2	000638-53-9	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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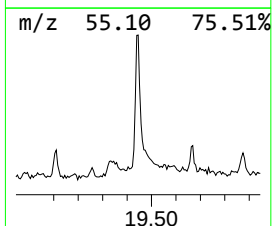
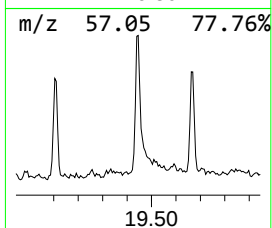
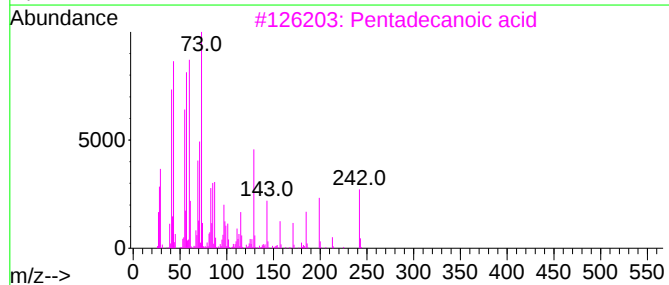
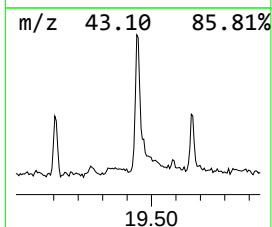
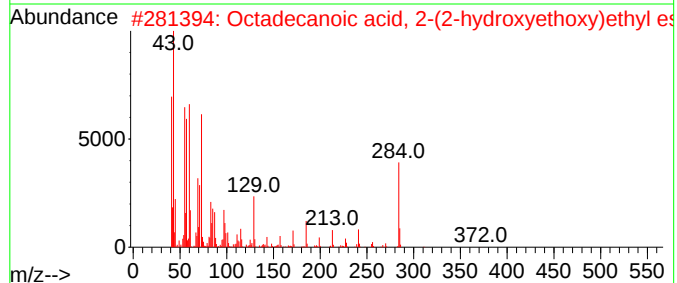
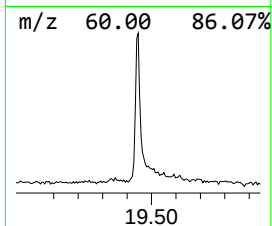
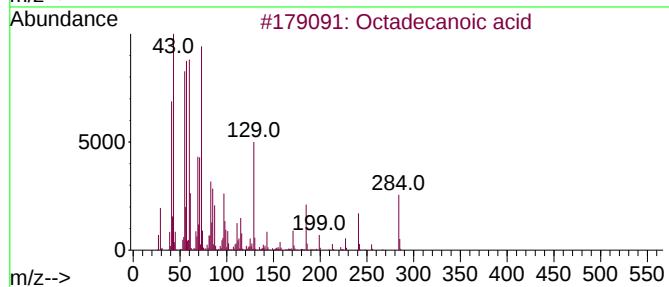
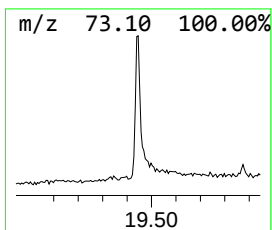
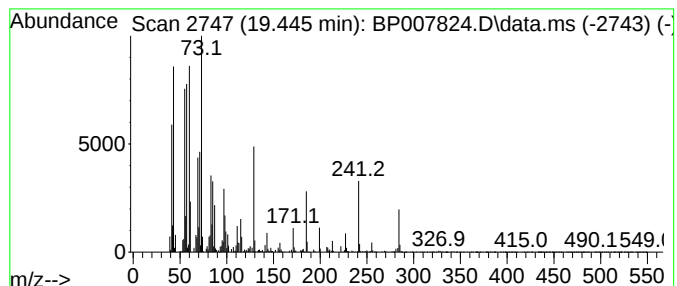
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	2.55 ng	576532	Chrysene-d12	21.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110321\
Data File : BP007824.D
Acq On : 03 Nov 2021 15:56
Operator : CG/JU
Sample : M4427-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

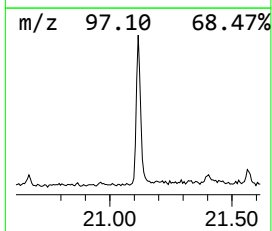
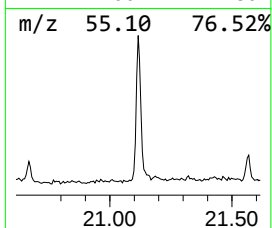
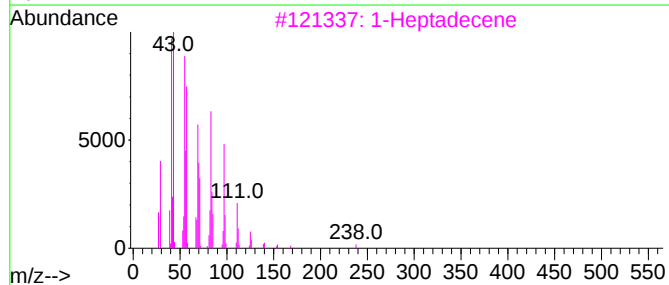
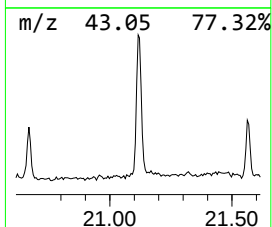
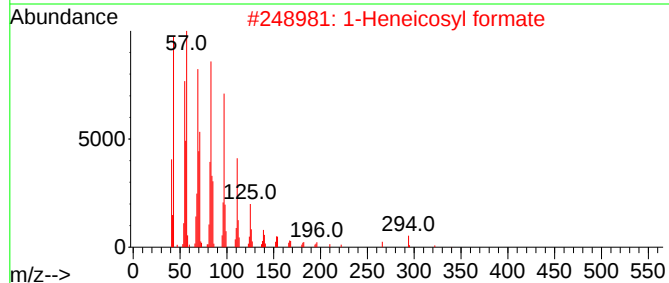
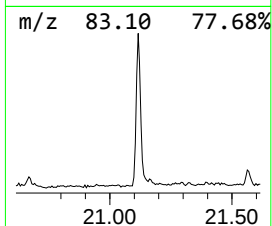
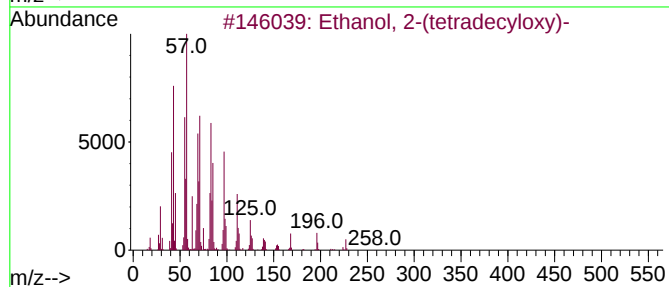
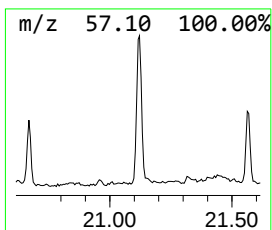
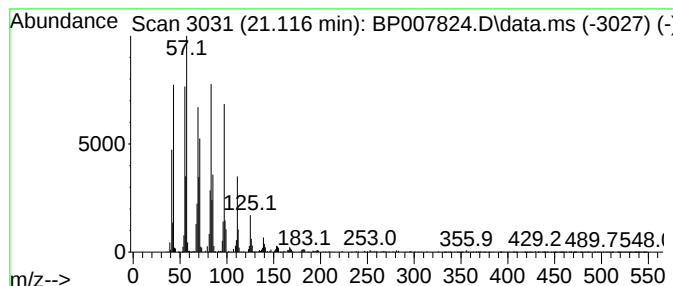
Instrument :
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ClientSampleId :
FDR-BH-6-20211029-7.5-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.116	4.21 ng	951617	Chrysene-d12		21.404	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-		258	C16H34O2	002136-70-1	97
2	1-Heneicosyl formate		340	C22H44O2	077899-03-7	97
3	1-Heptadecene		238	C17H34	006765-39-5	95
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	1-Hexacosanol		382	C26H54O	000506-52-5	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110321\
Data File : BP007824.D
Acq On : 03 Nov 2021 15:56
Operator : CG/JU
Sample : M4427-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FDR-BH-6-20211029-7.5-8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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, 1,3-di...	5.934	2.3	ng	140461	1	7.916	1220110	20.0
Ethanol, 2-(2-b...	10.505	7.4	ng	666046	2	10.722	1806940	20.0
unknown17.439	17.439	2.0	ng	332640	4	17.310	3256190	20.0
n-Hexadecanoic ...	18.210	7.1	ng	1152420	4	17.310	3256190	20.0
Octadecanoic acid	19.445	2.5	ng	576532	5	21.404	4517690	20.0
Ethanol, 2-(tet...	21.116	4.2	ng	951617	5	21.404	4517690	20.0