

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100220\
 Data File : BP003459.D
 Acq On : 02 Oct 2020 14:41
 Operator : CG/JU
 Sample : L4198-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 RO-15

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\8270-BP091520.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003459.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.140	377	383	420	rBV	1173234	2040552	39.08%	6.475%
2	6.734	647	654	678	rBV	1027468	2060469	39.46%	6.539%
3	7.528	782	789	801	rBV	366397	618341	11.84%	1.962%
4	8.681	977	985	1007	rBV	726688	1461398	27.99%	4.638%
5	10.305	1254	1261	1293	rBV	370096	878199	16.82%	2.787%
6	12.799	1678	1685	1711	rBV	1834288	3545753	67.91%	11.252%
7	13.651	1825	1830	1843	rBV	111204	233553	4.47%	0.741%
8	14.187	1914	1921	1942	rBV2	666982	1197830	22.94%	3.801%
9	15.692	2170	2177	2202	rBV	1222193	2419247	46.33%	7.677%
10	15.934	2214	2218	2233	rVB	65071	120009	2.30%	0.381%
11	16.728	2349	2353	2357	rBV	79082	96039	1.84%	0.305%
12	16.781	2358	2362	2368	rVB2	45390	69009	1.32%	0.219%
13	16.945	2384	2390	2396	rBV	888334	1447911	27.73%	4.595%
14	17.087	2410	2414	2420	rVB	30370	56076	1.07%	0.178%
15	17.469	2475	2479	2484	rBV	83728	98750	1.89%	0.313%
16	18.151	2590	2595	2598	rBV	75989	93956	1.80%	0.298%
17	18.763	2695	2699	2704	rBV2	70102	85876	1.64%	0.273%
18	18.863	2712	2716	2723	rVB	51154	78157	1.50%	0.248%
19	18.975	2730	2735	2743	rBV	429018	556357	10.66%	1.766%
20	19.298	2786	2790	2791	rBV	83701	90224	1.73%	0.286%
21	19.322	2791	2794	2798	rVV	325141	436086	8.35%	1.384%
22	19.528	2823	2829	2834	rBV2	3955554	5221311	100.00%	16.569%
23	19.651	2845	2850	2856	rVB3	41195	89808	1.72%	0.285%
24	19.781	2868	2872	2874	rBV3	39106	60210	1.15%	0.191%
25	19.816	2875	2878	2880	rVV	61664	73887	1.42%	0.234%
26	19.845	2880	2883	2886	rVB	61771	69659	1.33%	0.221%
27	19.910	2890	2894	2898	rBV	40919	52252	1.00%	0.166%
28	19.963	2898	2903	2907	rBV3	56126	100492	1.92%	0.319%
29	20.328	2960	2965	2968	rBV2	79954	103596	1.98%	0.329%
30	20.551	3000	3003	3007	rBV	61392	70728	1.35%	0.224%
31	20.704	3026	3029	3032	rBV	56007	81633	1.56%	0.259%
32	20.739	3032	3035	3037	rVV2	73444	89020	1.70%	0.282%
33	20.775	3037	3041	3047	rVV3	585078	913696	17.50%	2.900%
34	20.833	3047	3051	3061	rVB2	186102	330274	6.33%	1.048%
35	21.045	3081	3087	3092	rBV2	1433587	2218611	42.49%	7.041%
36	21.086	3092	3094	3103	rVB	233369	265838	5.09%	0.844%

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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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37	21.204	3110	3114	3117	rBV2	154455	183551	3.52%	0.582%
38	21.627	3182	3186	3195	rBV5	96607	204628	3.92%	0.649%
39	22.069	3257	3261	3274	rVB4	173431	295714	5.66%	0.938%
40	22.198	3279	3283	3293	rVB	226635	326671	6.26%	1.037%
41	22.580	3342	3348	3353	rBV2	302894	708345	13.57%	2.248%
42	23.045	3422	3427	3434	rVB	137642	232403	4.45%	0.738%
43	23.139	3437	3443	3451	rBV	175347	348541	6.68%	1.106%
44	23.233	3452	3459	3466	rBV2	957388	1787419	34.23%	5.672%

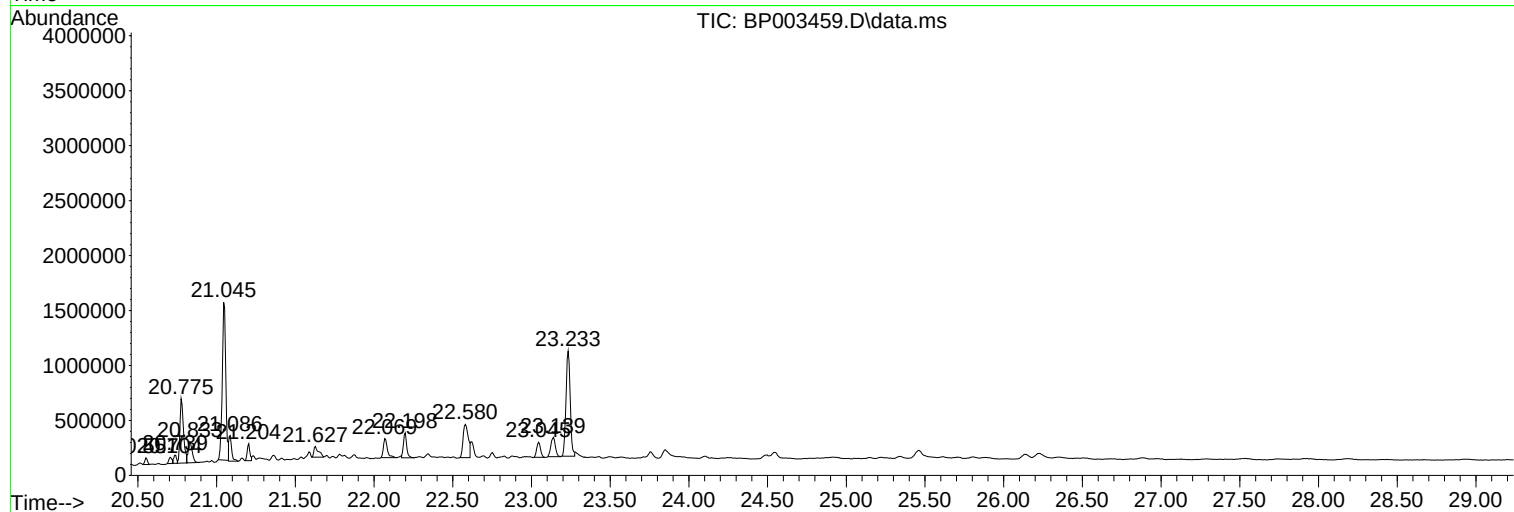
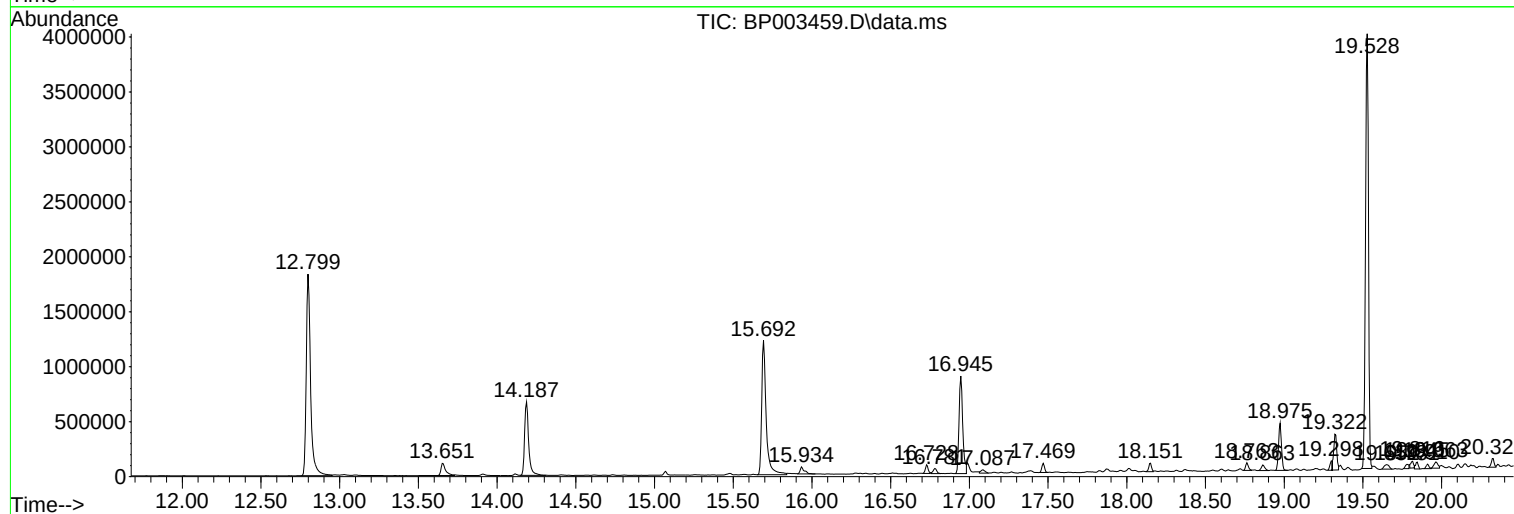
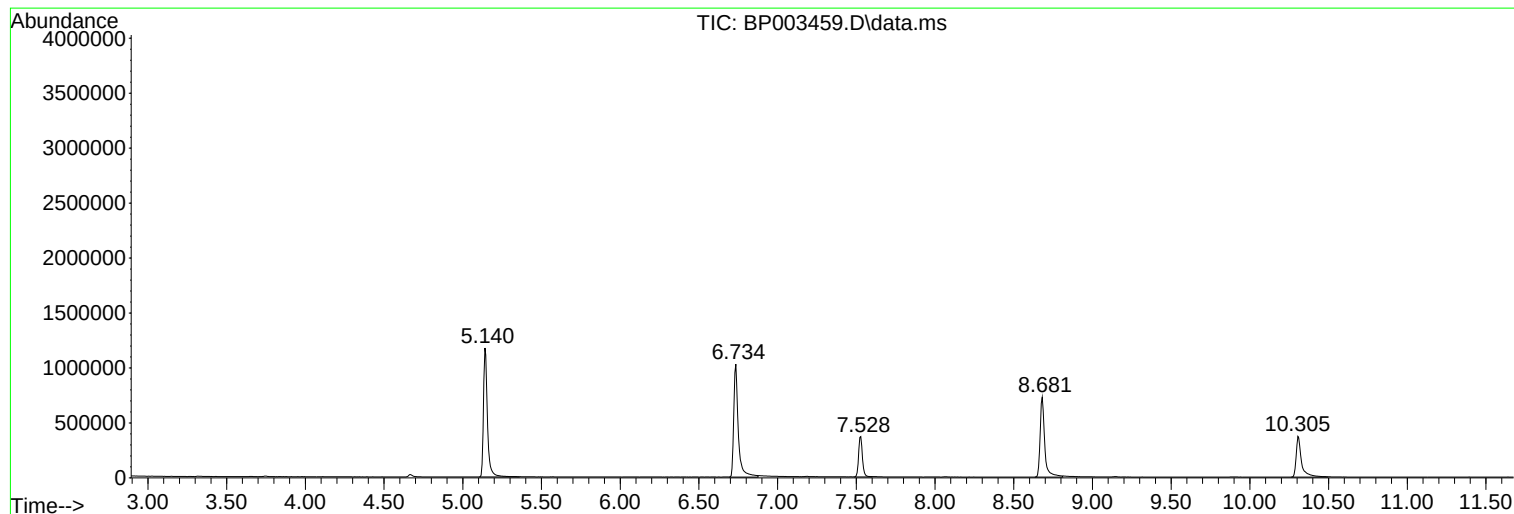
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : L4198-01
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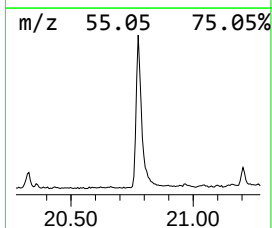
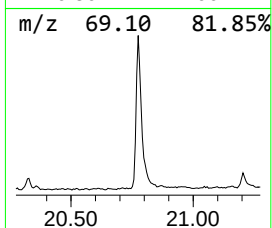
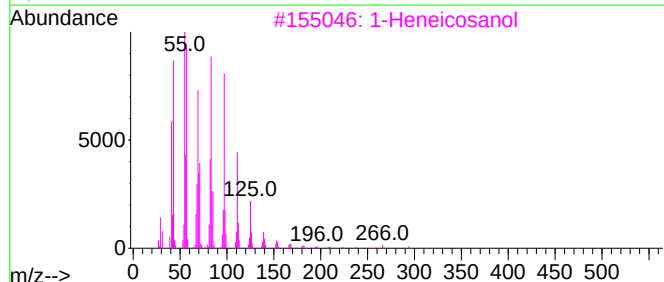
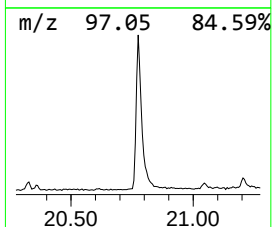
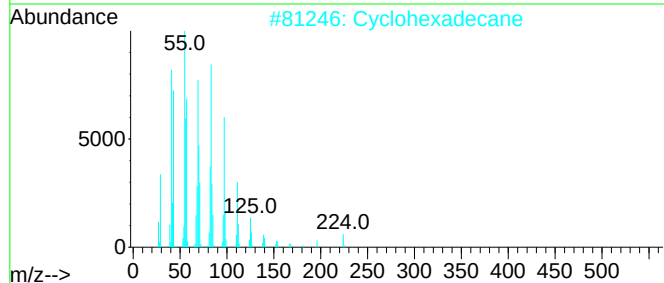
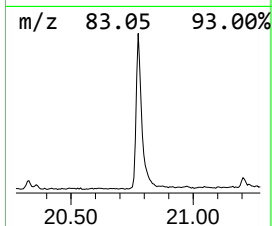
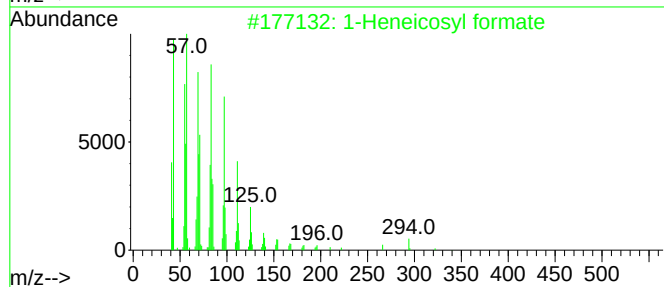
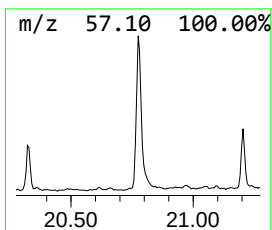
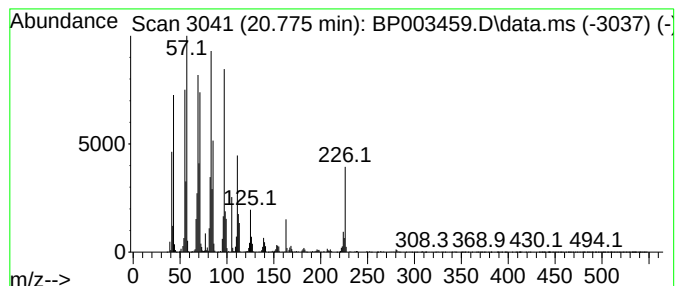
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Heneicosyl formate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.775	8.24 ng	913696	Chrysene-d12	21.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2			Cyclohexadecane	224	C16H32	000295-65-8	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	92
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	86



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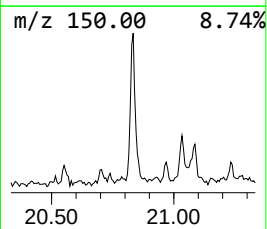
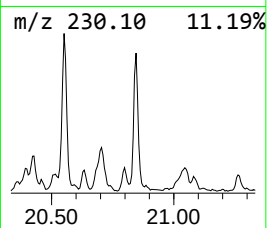
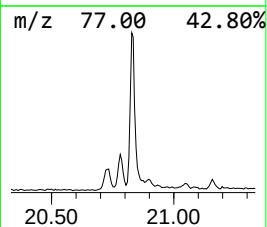
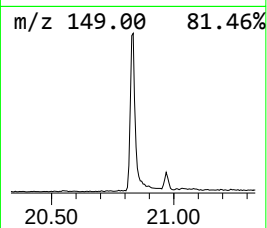
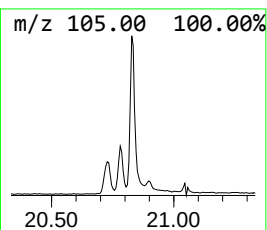
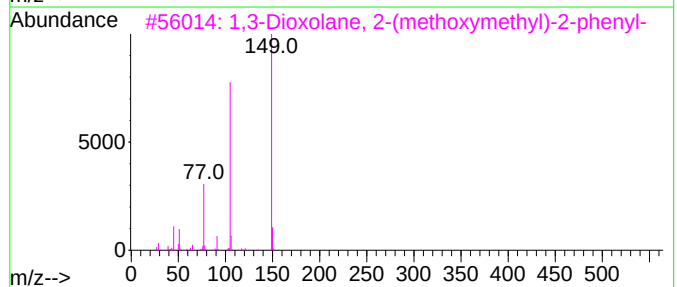
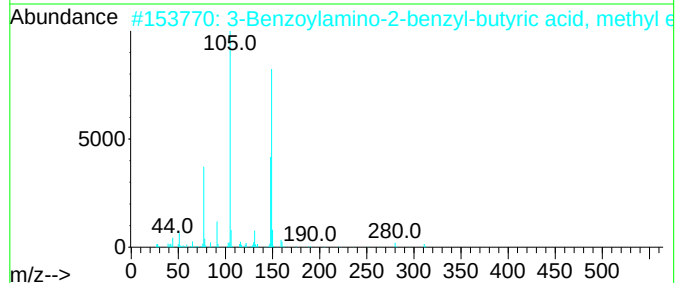
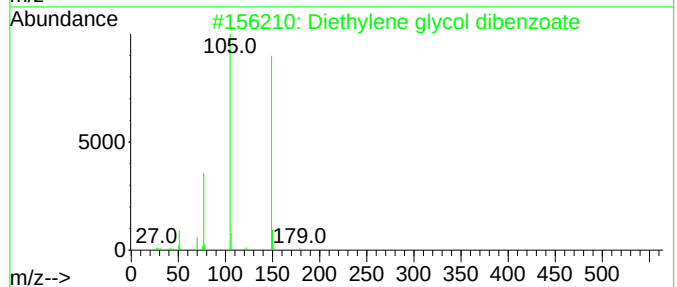
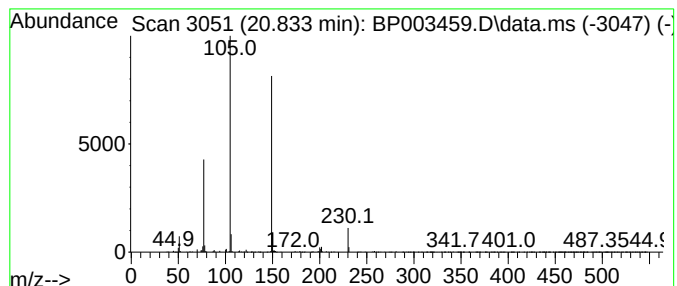
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.833	2.98 ng	330274	Chrysene-d12	21.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
2			3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	64
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	53
4			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	45
5			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	45



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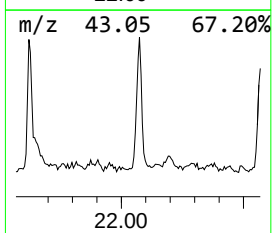
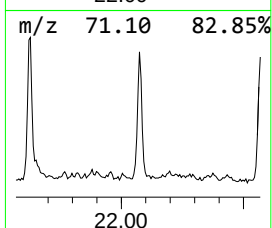
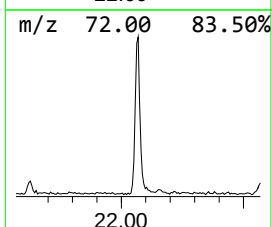
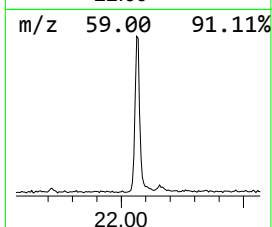
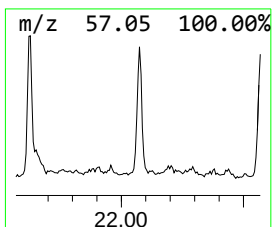
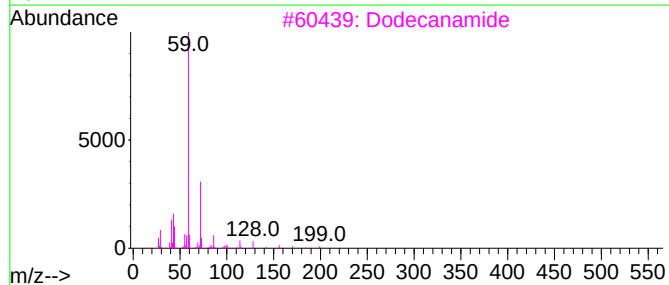
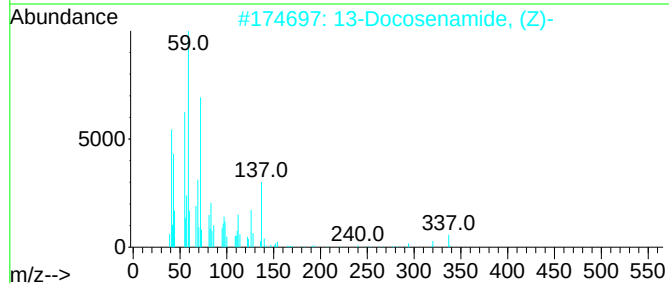
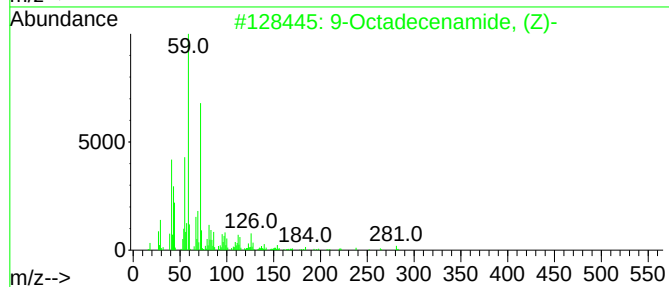
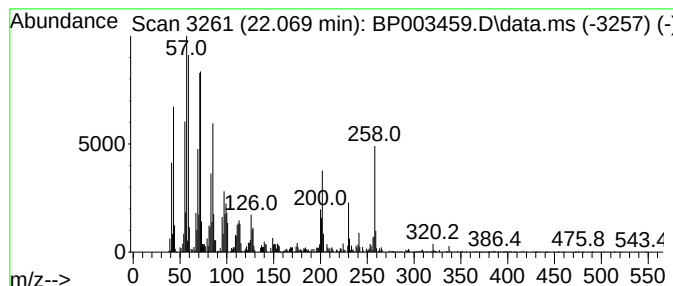
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown22.06 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.069	2.67 ng	295714	Chrysene-d12	21.045

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	38
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	14
3		Dodecanamide	199	C12H25NO	001120-16-7	14
4		Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	14
5		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	14



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Instrument :
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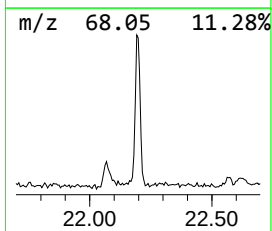
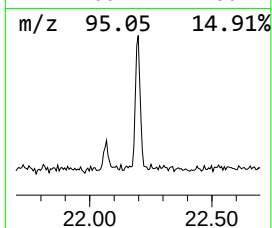
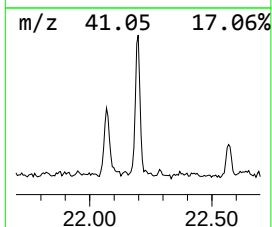
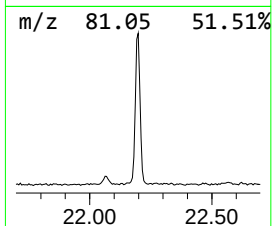
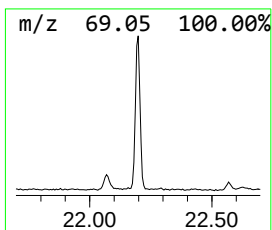
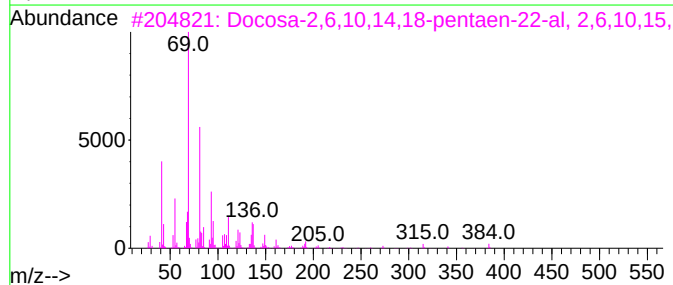
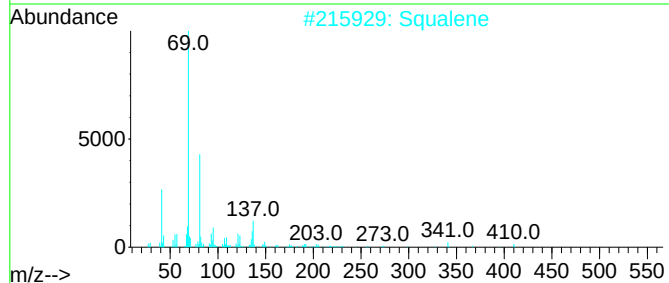
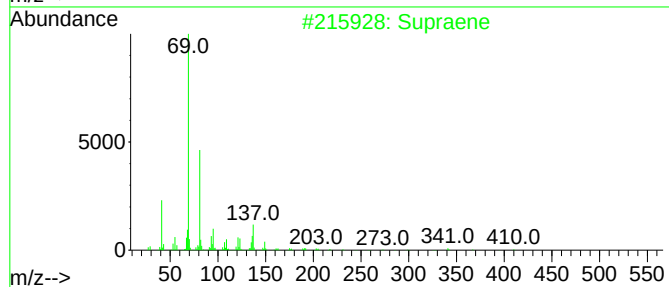
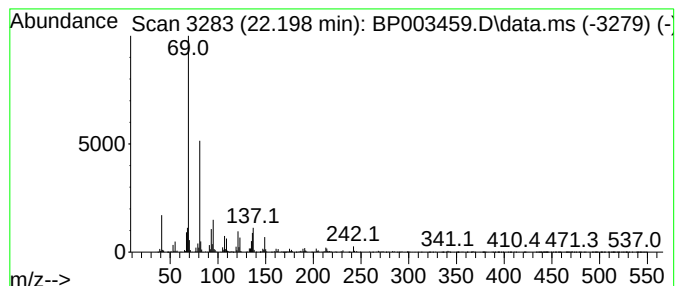
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.198	3.66 ng	326671	Perylene-d12	23.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	000762-29-8	64



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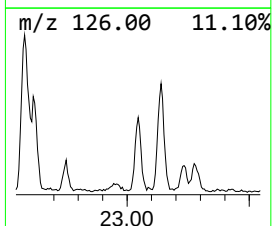
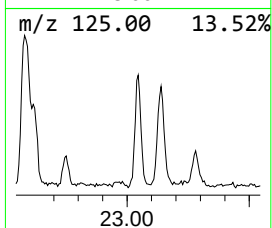
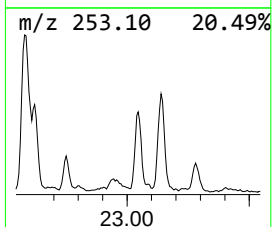
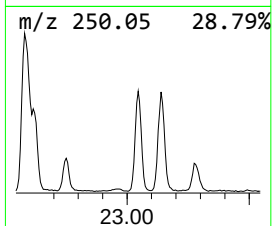
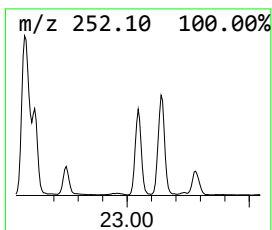
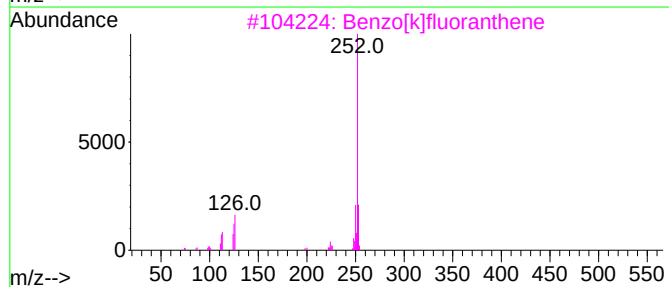
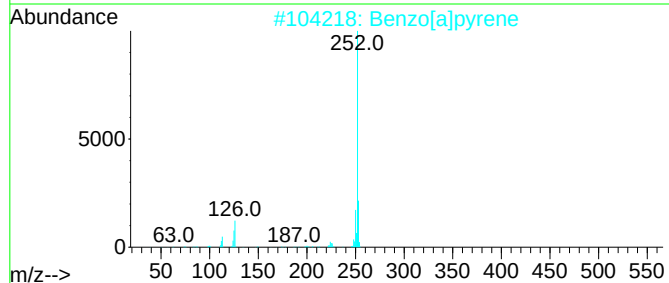
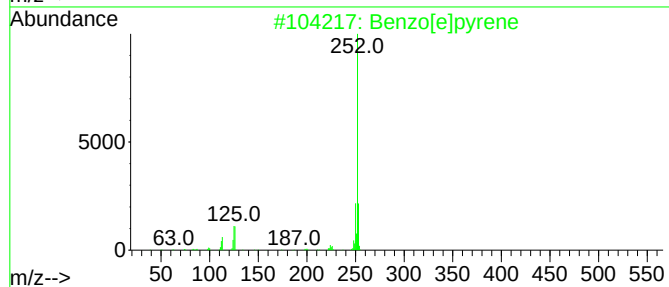
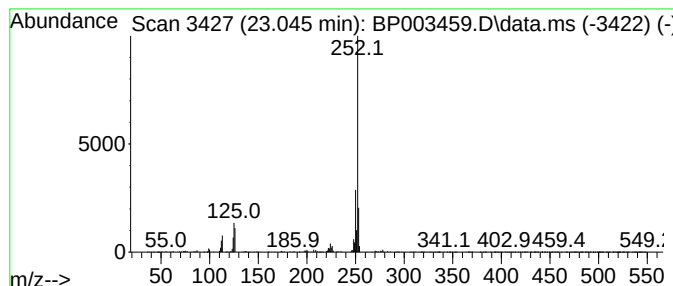
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.045	2.60 ng	232403	Perylene-d12	23.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	97
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
4			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
5			Perylene	252	C20H12	000198-55-0	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100220\
Data File : BP003459.D
Acq On : 02 Oct 2020 14:41
Operator : CG/JU
Sample : L4198-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.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
1-Heneicosyl fo...	20.775	8.2	ng	913696	5	21.045	2218610	20.0
Diethylene glyc...	20.833	3.0	ng	330274	5	21.045	2218610	20.0
unknown22.06	22.069	2.7	ng	295714	5	21.045	2218610	20.0
Supraene	22.198	3.7	ng	326671	6	23.233	1787420	20.0
Benzo[e]pyrene	23.045	2.6	ng	232403	6	23.233	1787420	20.0