

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
 Data File : BP007154.D
 Acq On : 24 Sep 2021 12:17
 Operator : CG/JU
 Sample : M3823-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DKM-ENV-IG

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-BP092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007154.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.464	397	404	416	rBV	2763304	4002178	4.13%	1.781%
2	7.058	667	675	689	rBV	2471100	4014889	4.15%	1.787%
3	7.887	810	816	823	rVB	815854	1282545	1.33%	0.571%
4	9.052	1005	1014	1027	rBV	1539828	2574075	2.66%	1.145%
5	10.693	1285	1293	1300	rVB	1038292	1755920	1.81%	0.781%
6	13.145	1703	1710	1719	rBV	4079498	6222548	6.43%	2.769%
7	14.522	1937	1944	1952	rBV	1622088	2342013	2.42%	1.042%
8	16.010	2192	2197	2206	rVB	3243228	4635897	4.79%	2.063%
9	16.586	2261	2295	2297	rBV2	3465419	20882022	21.57%	9.292%
10	16.892	2324	2347	2369	rVB2	5615473	38084014	39.35%	16.947%
11	17.216	2371	2402	2410	rBV	13952979	96792431	100.00%	43.071%
12	17.428	2424	2438	2459	rVB	1994530	7510979	7.76%	3.342%
13	18.163	2557	2563	2583	rBV	1888160	2993832	3.09%	1.332%
14	18.557	2623	2630	2645	rVB	413695	1229302	1.27%	0.547%
15	19.680	2815	2821	2832	rVB	854694	1785566	1.84%	0.795%
16	19.833	2841	2847	2852	rBV	7349095	8897435	9.19%	3.959%
17	20.539	2961	2967	2975	rVB	829664	1871052	1.93%	0.833%
18	21.263	3085	3090	3097	rBV	1291457	2217168	2.29%	0.987%
19	21.357	3102	3106	3111	rVB	2335150	3039693	3.14%	1.353%
20	21.992	3208	3214	3221	rVB	1016356	2110934	2.18%	0.939%
21	22.786	3344	3349	3357	rVB	792640	1743414	1.80%	0.776%
22	22.886	3360	3366	3380	rVB	1142455	3042292	3.14%	1.354%
23	23.080	3394	3399	3407	rVB2	1139212	2517787	2.60%	1.120%
24	23.774	3512	3517	3525	rVB2	1568259	3177983	3.28%	1.414%

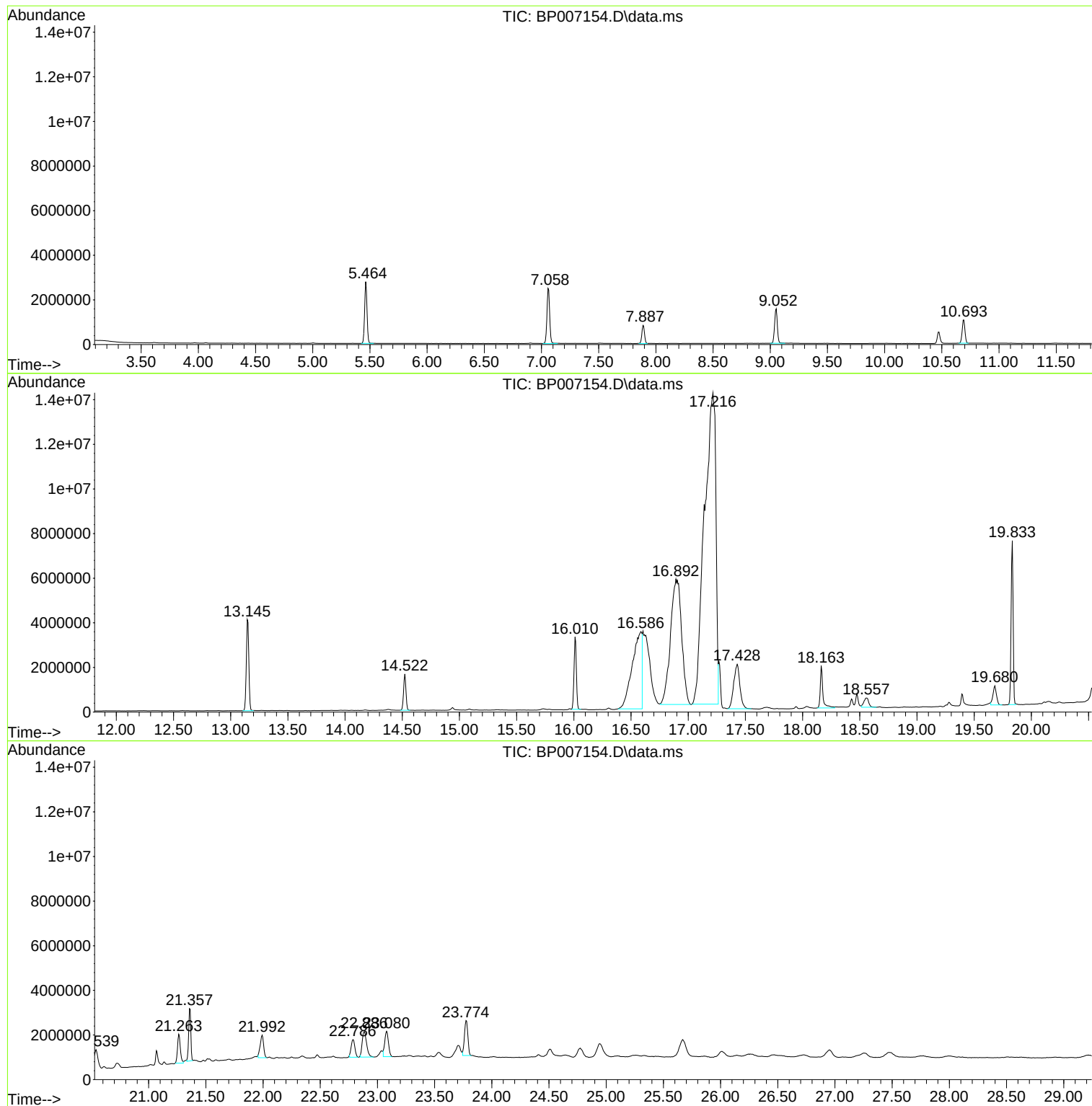
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BP007154.D
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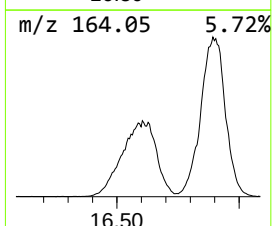
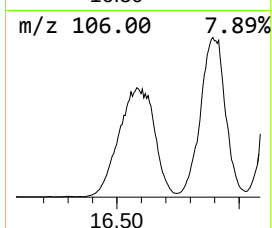
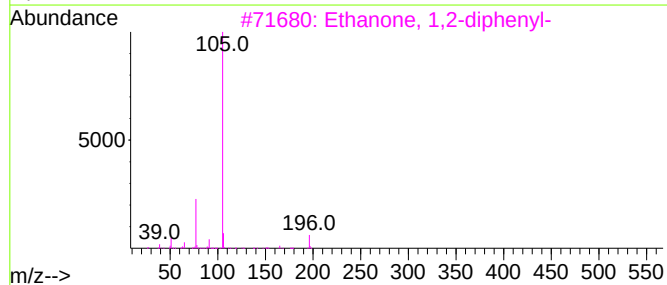
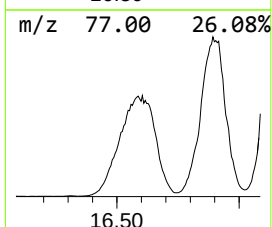
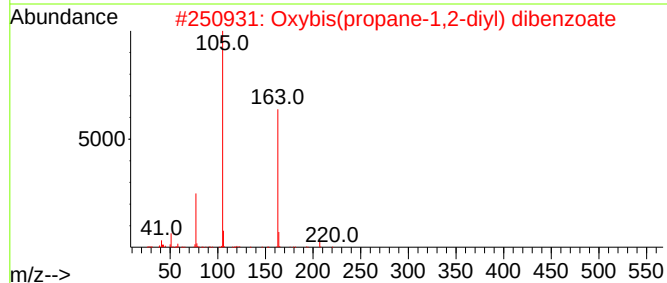
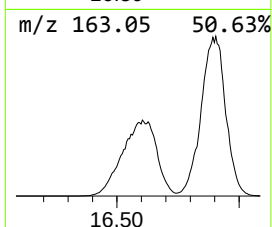
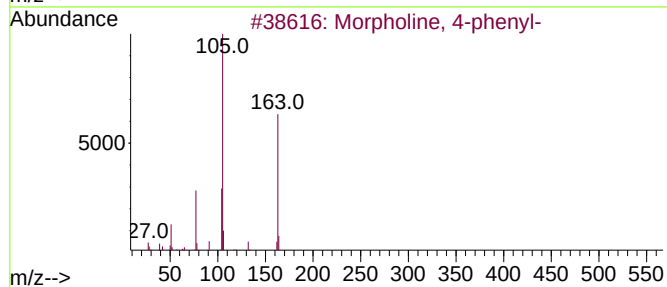
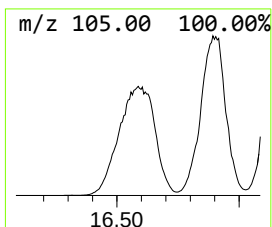
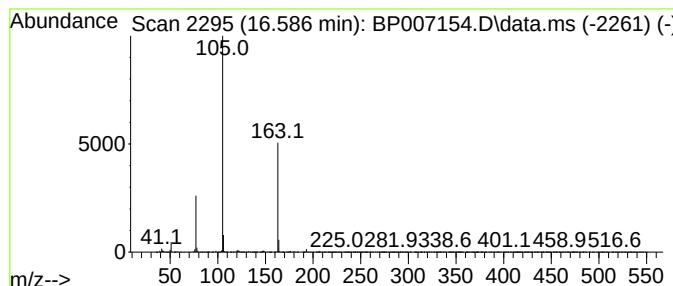
Instrument :
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ClientSampleId :
DKM-ENV-IG

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Oxybis(propene-1,2-diyl) di... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.587	4.31 ng	20882000	Phenanthrene-d10	17.275	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
3	Ethanone, 1,2-diphenyl-	196	C14H12O	000451-40-1	38
4	Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38
5	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	38



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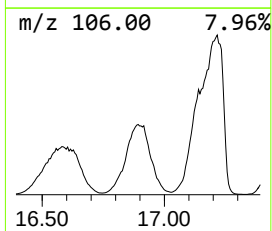
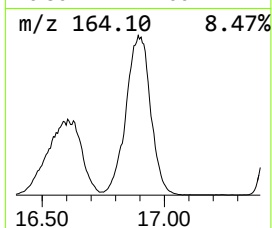
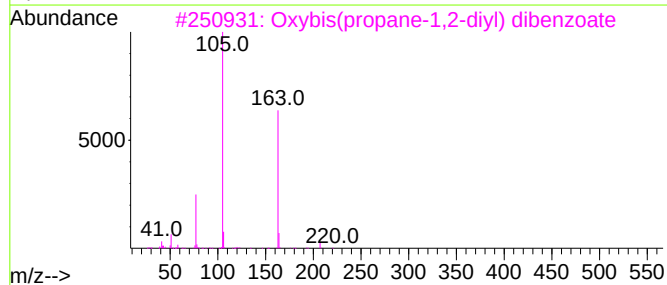
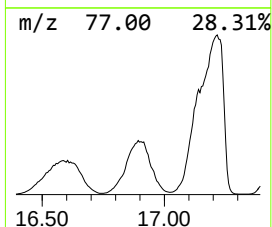
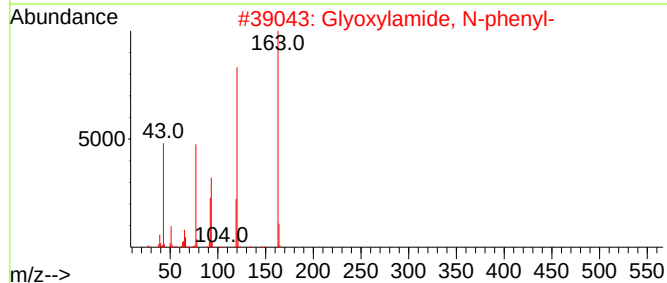
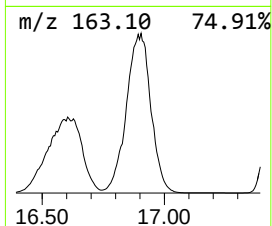
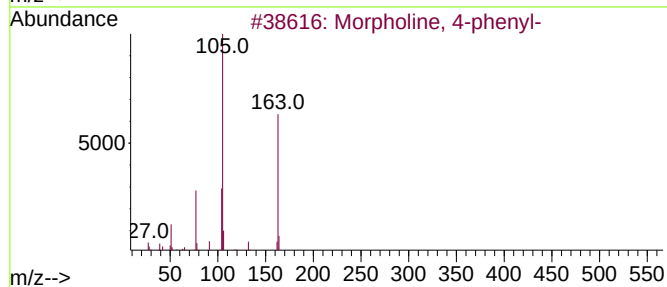
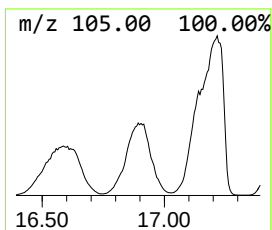
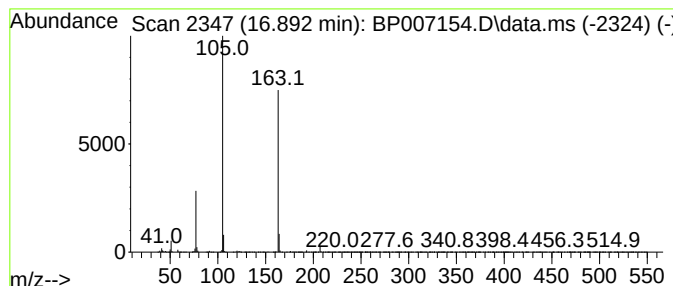
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Morpholine, 4-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.892	7.87 ng	38084000	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	78
2			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	59
3			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	43
4			Phenylglyoxylic acid, propyl ester	192	C11H12O3	1000453-46-7	22
5			Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	22



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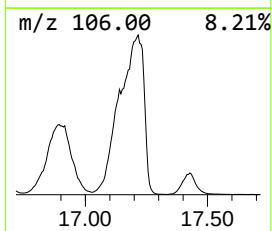
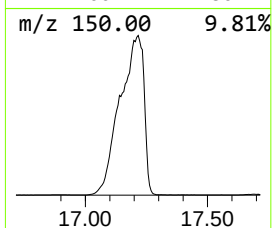
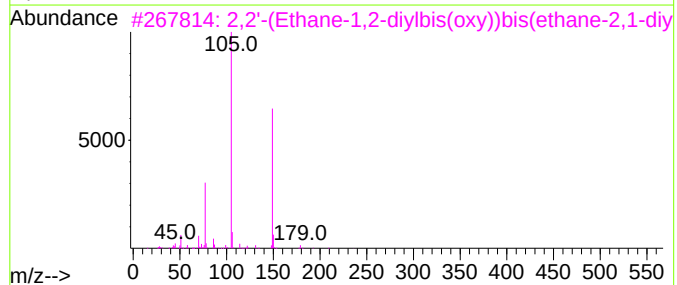
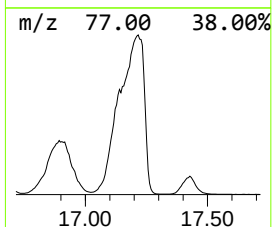
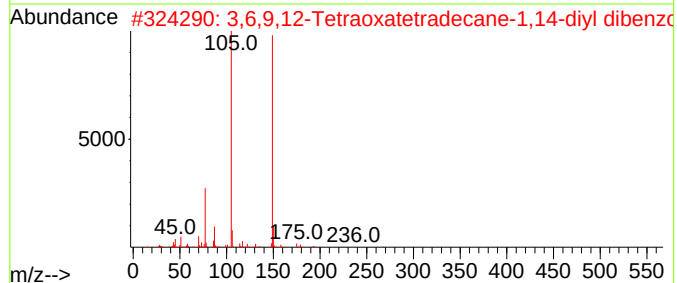
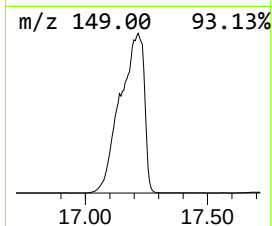
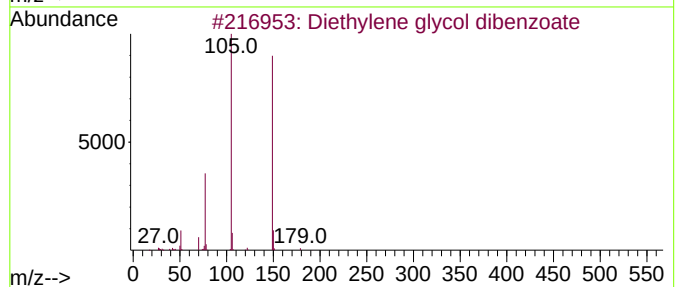
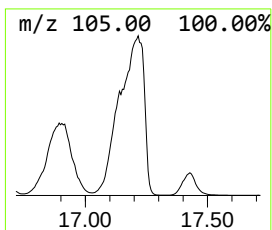
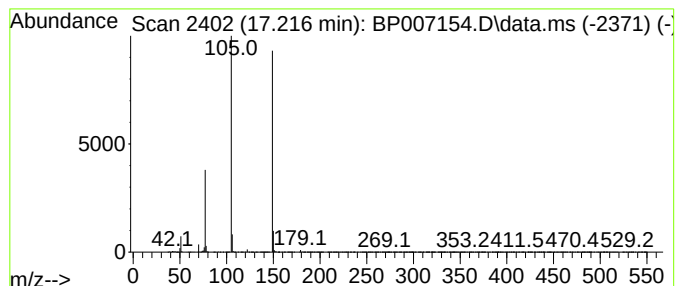
Instrument :
BNA_P
ClientSampleId :
DKM-ENV-IG

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

Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.216	20.00 ng	96792400	Phenanthrene-d10	17.275	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	83
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	78
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DKM-ENV-IG

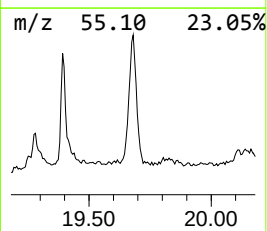
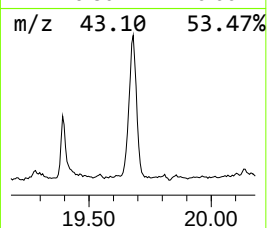
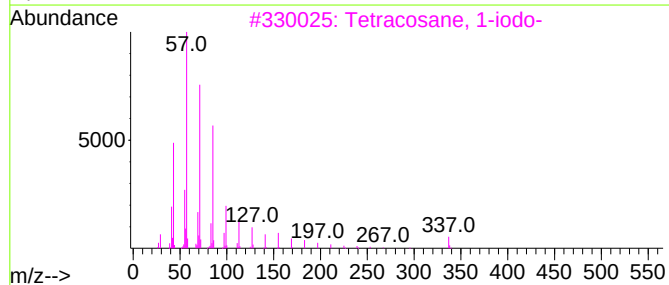
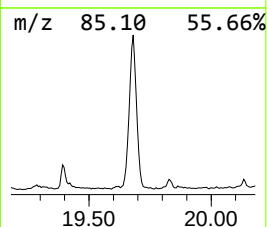
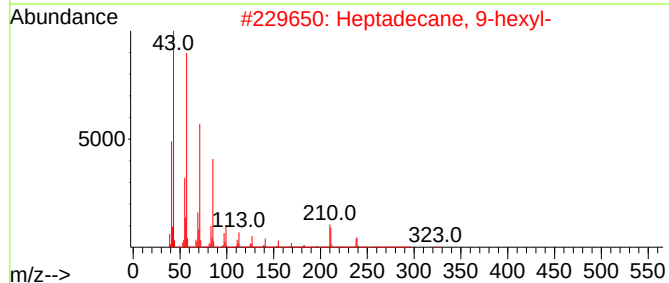
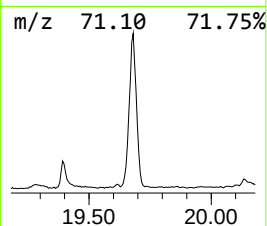
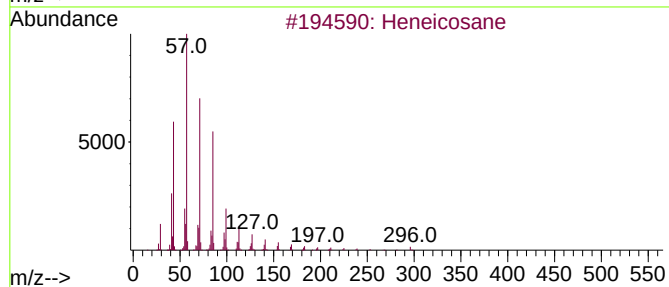
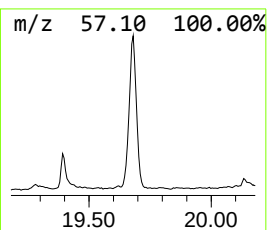
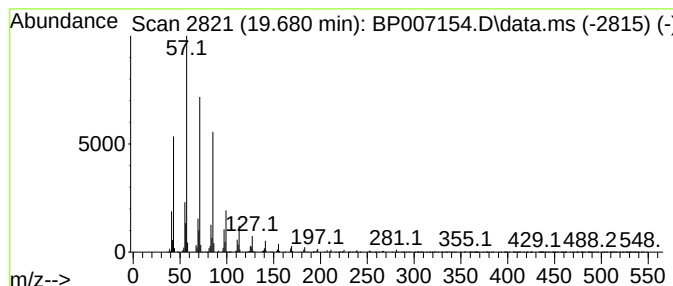
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Peak Number 4 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.680	11.75 ng	1785570	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91
4			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	91



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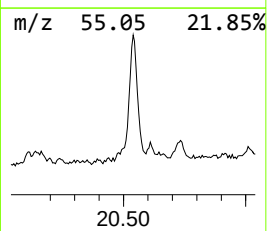
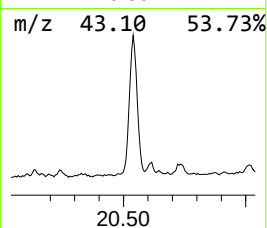
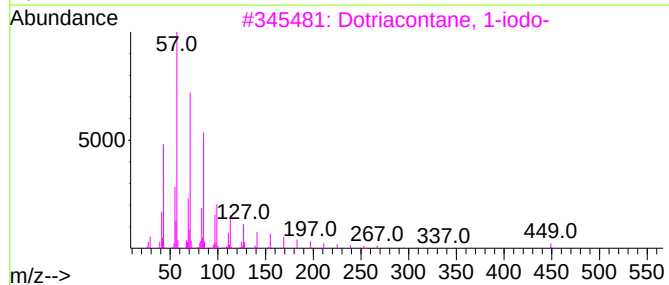
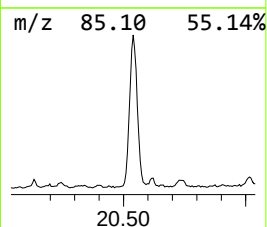
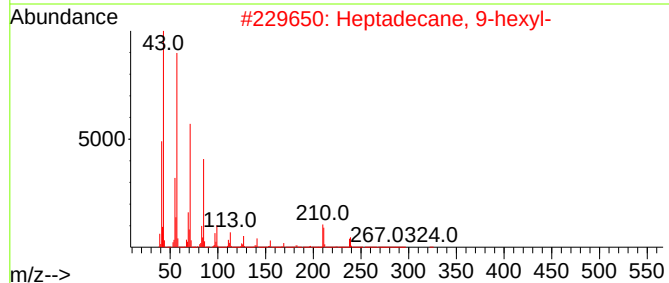
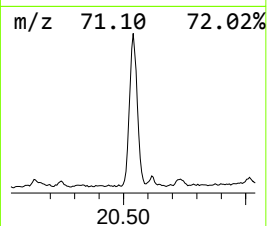
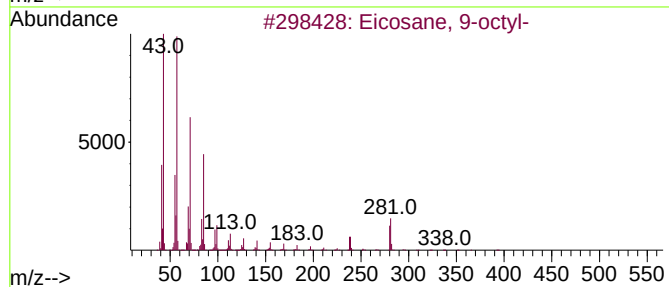
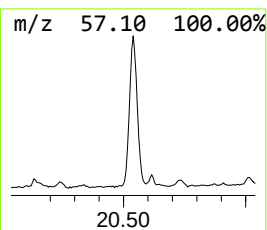
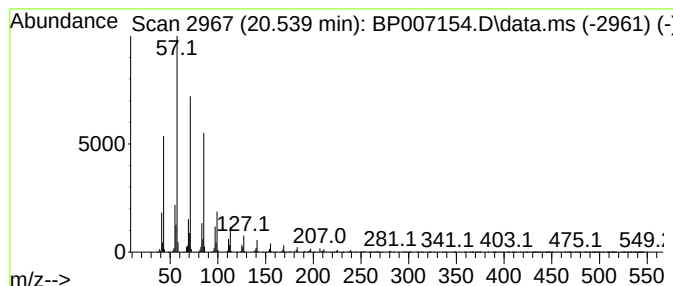
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.539	12.31 ng	1871050	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 9-octyl-	394	C28H58	013475-77-9	94
2			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Octacosane	394	C28H58	000630-02-4	91



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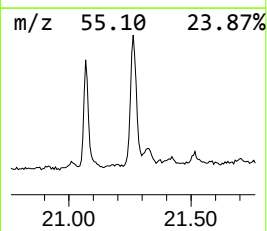
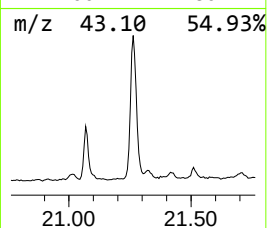
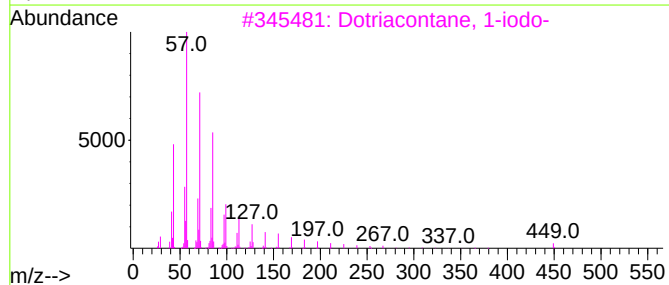
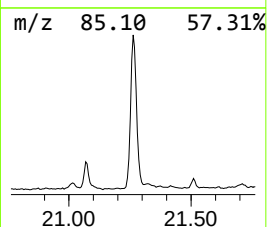
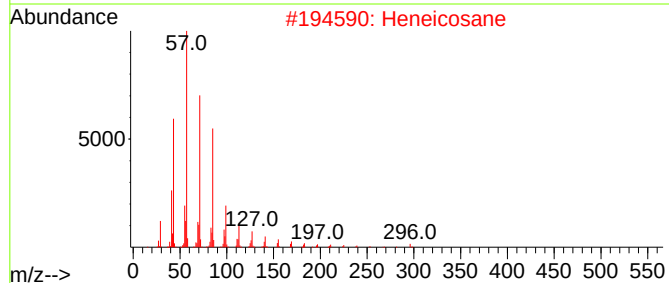
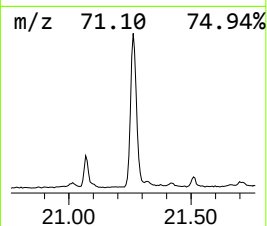
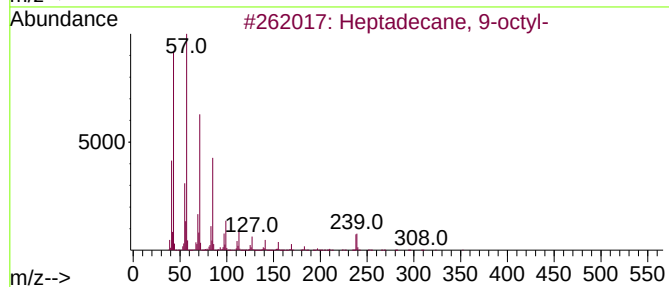
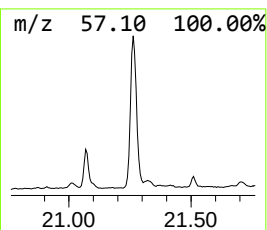
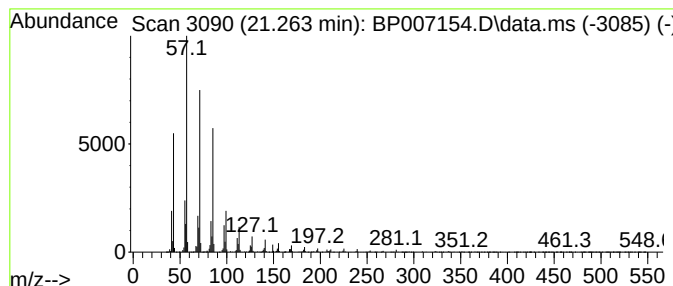
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.263	14.59 ng	2217170	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2			Heneicosane	296	C21H44	000629-94-7	91
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			1,3-Propanediol, eicosyl ethyl e...	384	C25H52O2	1000406-35-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007154.D
Acq On : 24 Sep 2021 12:17
Operator : CG/JU
Sample : M3823-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DKM-ENV-IG

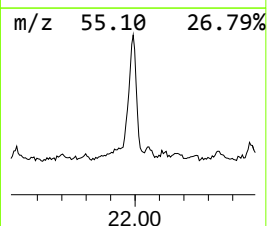
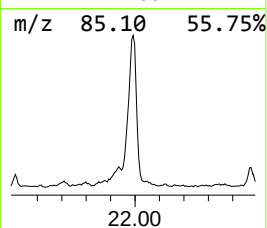
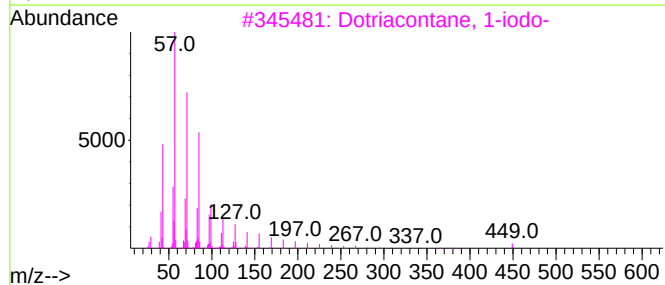
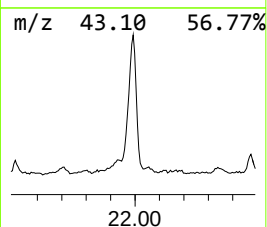
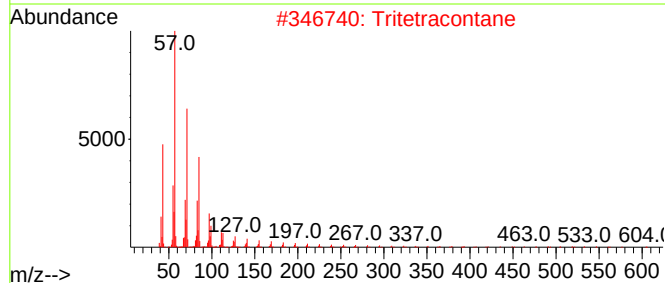
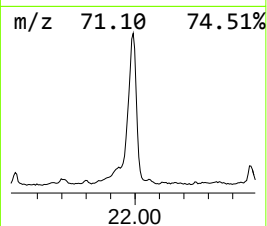
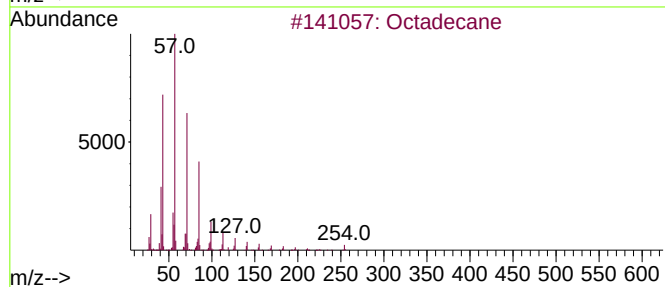
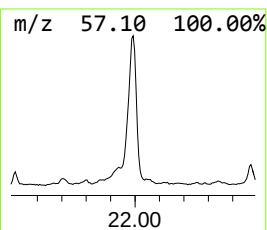
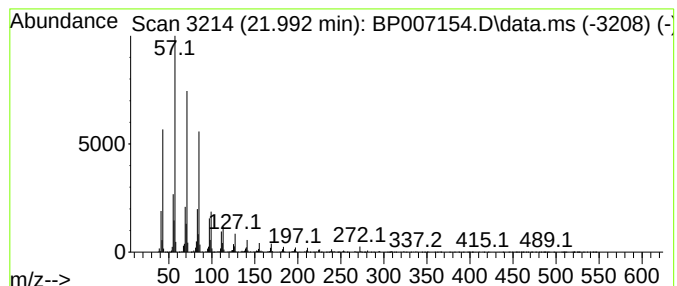
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.992	13.89 ng	2110930	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Tritetracontane	605	C43H88	007098-21-7	91
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007154.D
Acq On : 24 Sep 2021 12:17
Operator : CG/JU
Sample : M3823-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DKM-ENV-IG

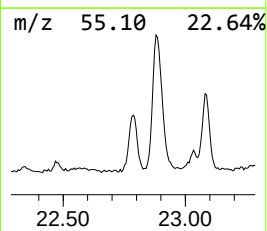
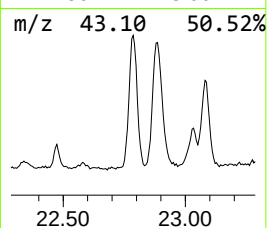
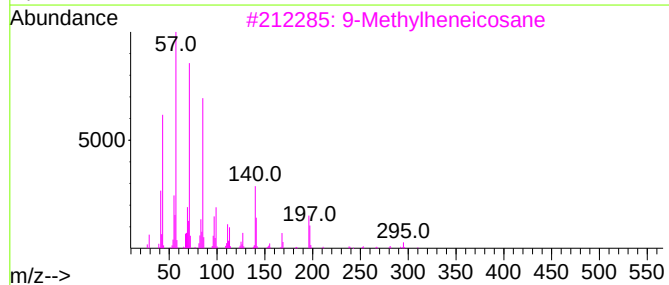
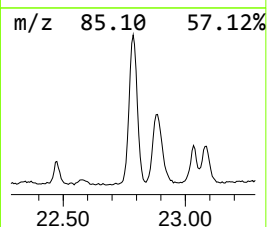
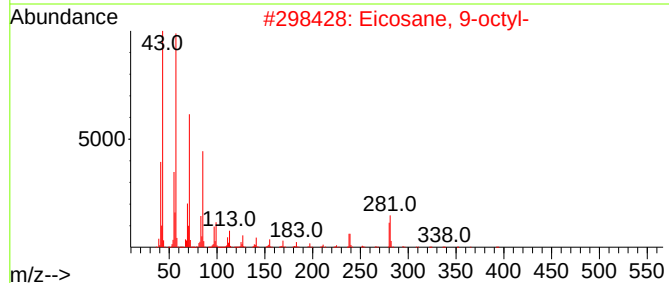
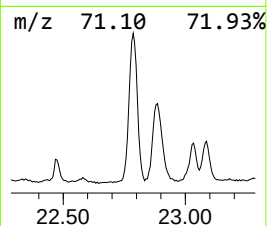
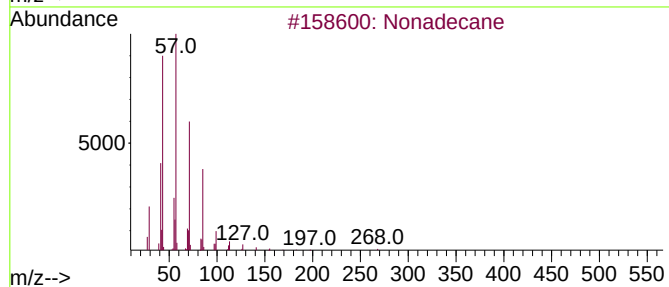
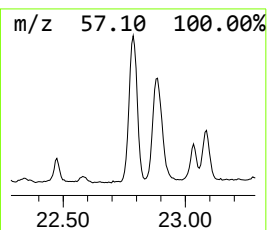
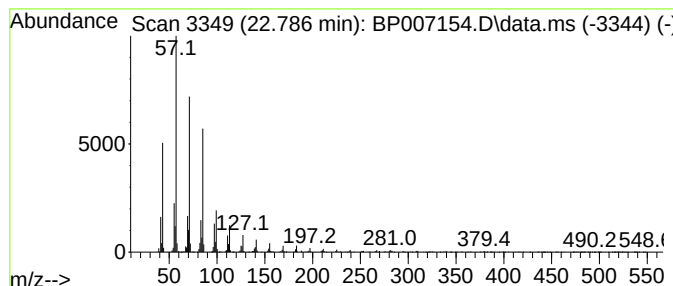
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.786	10.97 ng	1743410	Perylene-d12	23.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	94
2			Eicosane, 9-octyl-	394	C28H58	013475-77-9	93
3			9-Methylheneicosane	310	C22H46	070475-51-3	93
4			Heneicosane	296	C21H44	000629-94-7	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007154.D
Acq On : 24 Sep 2021 12:17
Operator : CG/JU
Sample : M3823-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DKM-ENV-IG

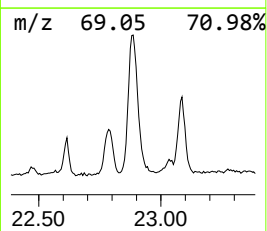
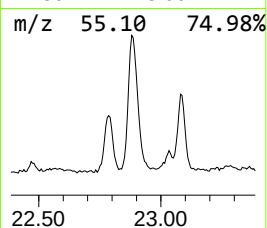
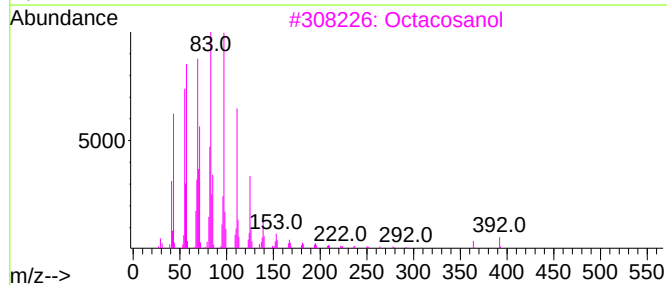
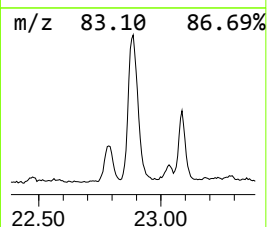
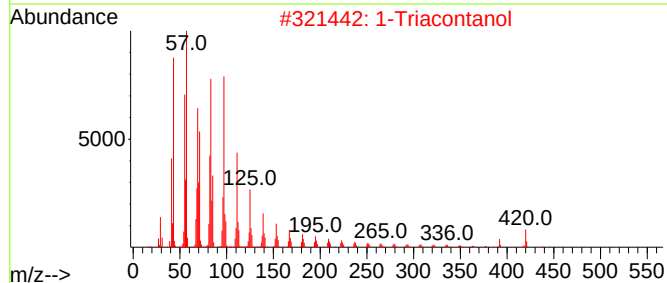
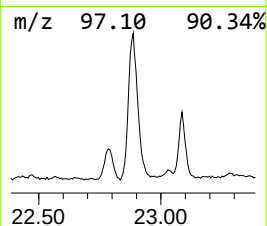
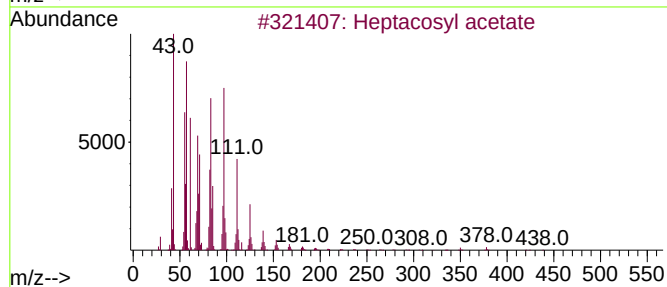
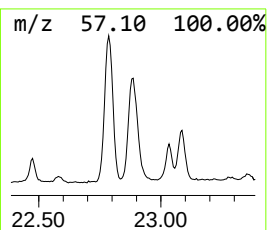
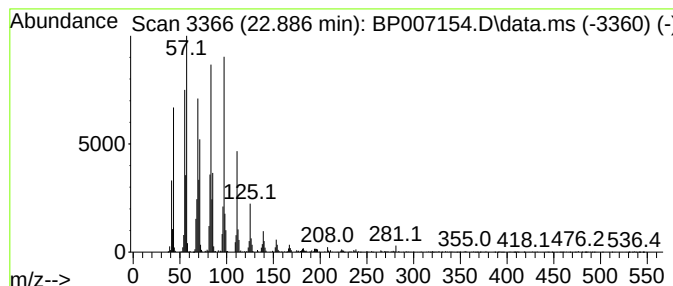
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.886	19.15 ng	3042290	Perylene-d12	23.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	97
2			1-Triacontanol	438	C30H62O	000593-50-0	96
3			Octacosanol	410	C28H58O	000557-61-9	94
4			Ethyl triacontyl ether	467	C32H66O	1000406-37-1	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007154.D
Acq On : 24 Sep 2021 12:17
Operator : CG/JU
Sample : M3823-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DKM-ENV-IG

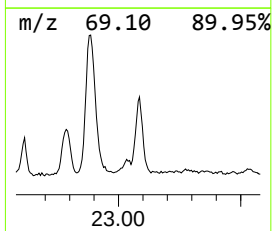
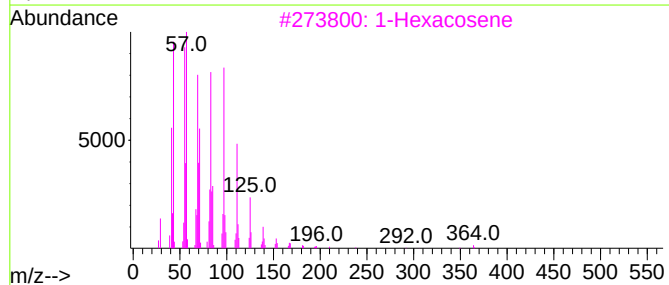
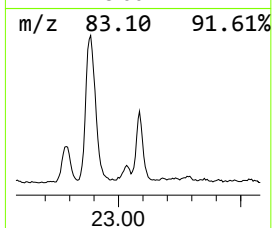
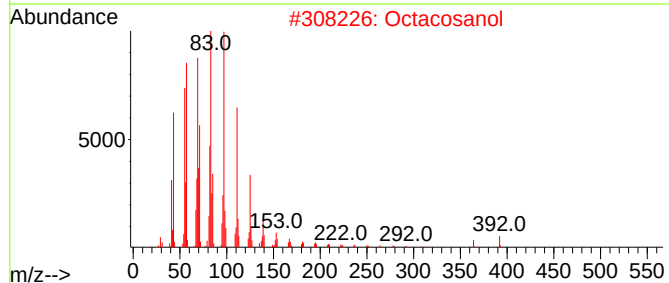
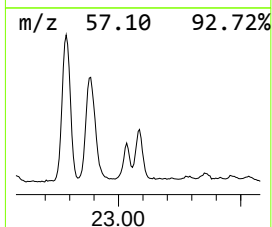
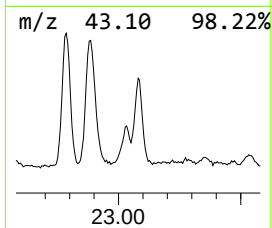
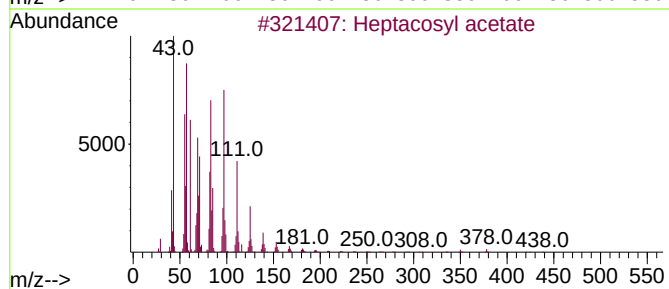
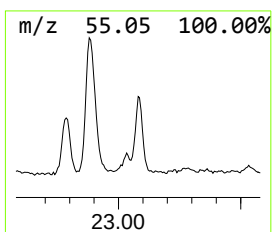
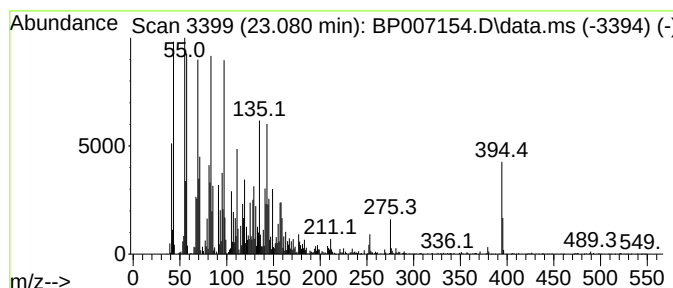
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.080	15.85 ng	2517790	Perylene-d12	23.774

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosyl acetate	438	C29H58O2	1000351-78-2	92
2		Octacosanol	410	C28H58O	000557-61-9	90
3		1-Hexacosene	364	C26H52	018835-33-1	90
4		Behenic alcohol	326	C22H46O	000661-19-8	62
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092421\
Data File : BP007154.D
Acq On : 24 Sep 2021 12:17
Operator : CG/JU
Sample : M3823-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DKM-ENV-IG

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.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
Oxybis(propane-...	16.587	4.3	ng	20882000	4	17.275	96792400	20.0
Morpholine, 4-p...	16.892	7.9	ng	38084000	4	17.275	96792400	20.0
Diethylene glyc...	17.216	20.0	ng	96792400	4	17.275	96792400	20.0
Heneicosane	19.680	11.8	ng	1785570	5	21.357	3039690	20.0
Eicosane, 9-octyl-	20.539	12.3	ng	1871050	5	21.357	3039690	20.0
Heptadecane, 9-...	21.263	14.6	ng	2217170	5	21.357	3039690	20.0
Octadecane	21.992	13.9	ng	2110930	5	21.357	3039690	20.0
Nonadecane	22.786	11.0	ng	1743410	6	23.774	3177980	20.0
Heptacosyl acetate	22.886	19.1	ng	3042290	6	23.774	3177980	20.0
Octacosanol	23.080	15.9	ng	2517790	6	23.774	3177980	20.0