

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
 Data File : BP004730.D
 Acq On : 12 Feb 2021 15:16
 Operator : CG/JU
 Sample : M1396-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 FK-BPM-04-013-ABCD

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-BP020521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004730.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.358	361	369	378	rBV	803498	1119978	43.81%	6.927%
2	6.940	630	638	648	rBV	735410	1180823	46.19%	7.303%
3	7.769	772	779	785	rBV	192490	300125	11.74%	1.856%
4	8.928	967	976	987	rBV	427508	723095	28.29%	4.472%
5	10.563	1247	1254	1261	rBV	236480	389349	15.23%	2.408%
6	13.040	1668	1675	1681	rBV	1096472	1577651	61.72%	9.758%
7	13.875	1807	1817	1824	rBV	49479	82666	3.23%	0.511%
8	14.157	1861	1865	1876	rBV3	12513	34964	1.37%	0.216%
9	14.416	1903	1909	1917	rVB2	357432	528343	20.67%	3.268%
10	14.981	2000	2005	2011	rVB2	20725	35269	1.38%	0.218%
11	15.628	2108	2115	2124	rVB	24324	63089	2.47%	0.390%
12	15.910	2157	2163	2170	rVB	985154	1355815	53.04%	8.386%
13	16.210	2209	2214	2223	rVB4	28325	51387	2.01%	0.318%
14	16.569	2268	2275	2283	rVB6	32687	84908	3.32%	0.525%
15	17.169	2372	2377	2384	rBV	462994	649150	25.39%	4.015%
16	18.069	2523	2530	2540	rBV	537593	737813	28.86%	4.563%
17	18.333	2569	2575	2578	rBV	89248	132633	5.19%	0.820%
18	18.375	2578	2582	2594	rVB3	70338	146485	5.73%	0.906%
19	19.163	2712	2716	2717	rBV2	41645	48148	1.88%	0.298%
20	19.186	2718	2720	2729	rVB2	46264	75546	2.96%	0.467%
21	19.304	2735	2740	2754	rVB2	404484	560200	21.92%	3.465%
22	19.739	2808	2814	2819	rBV	2155801	2556217	100.00%	15.810%
23	20.198	2884	2892	2908	rVB5	121733	508908	19.91%	3.148%
24	20.974	3020	3024	3033	rBV	141770	223347	8.74%	1.381%
25	21.257	3067	3072	3076	rBV	632516	788467	30.85%	4.877%
26	21.316	3076	3082	3096	rVB4	321681	1094330	42.81%	6.768%
27	21.639	3132	3137	3149	rVB3	126764	363265	14.21%	2.247%
28	23.568	3458	3465	3474	rVB2	386305	756424	29.59%	4.678%

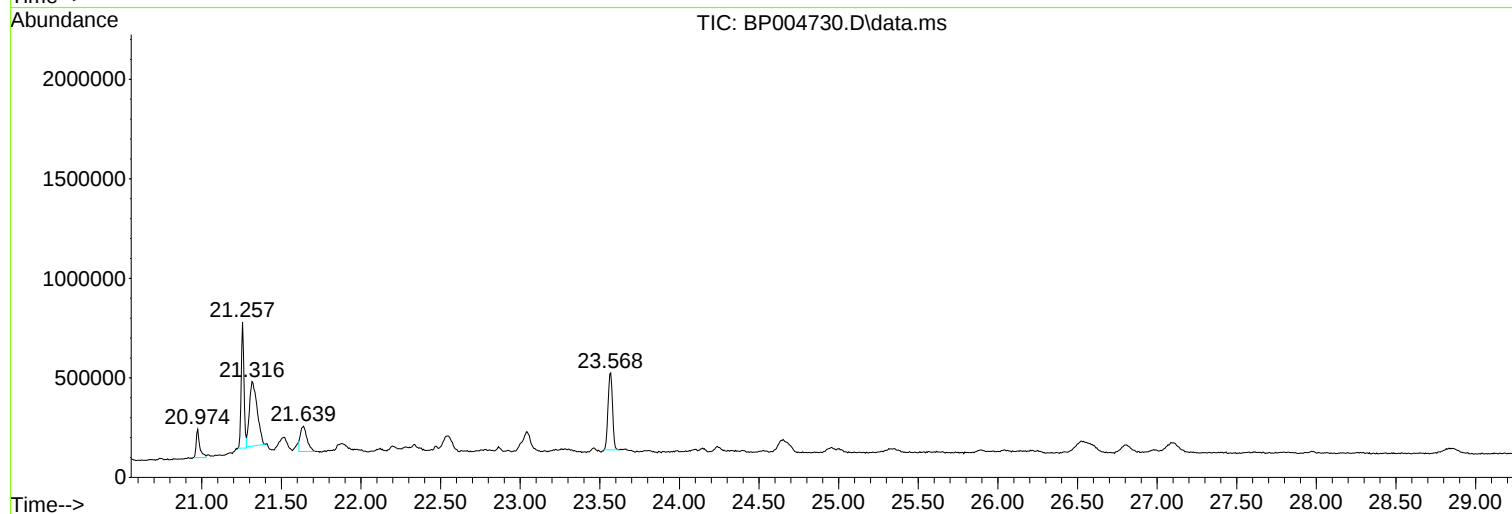
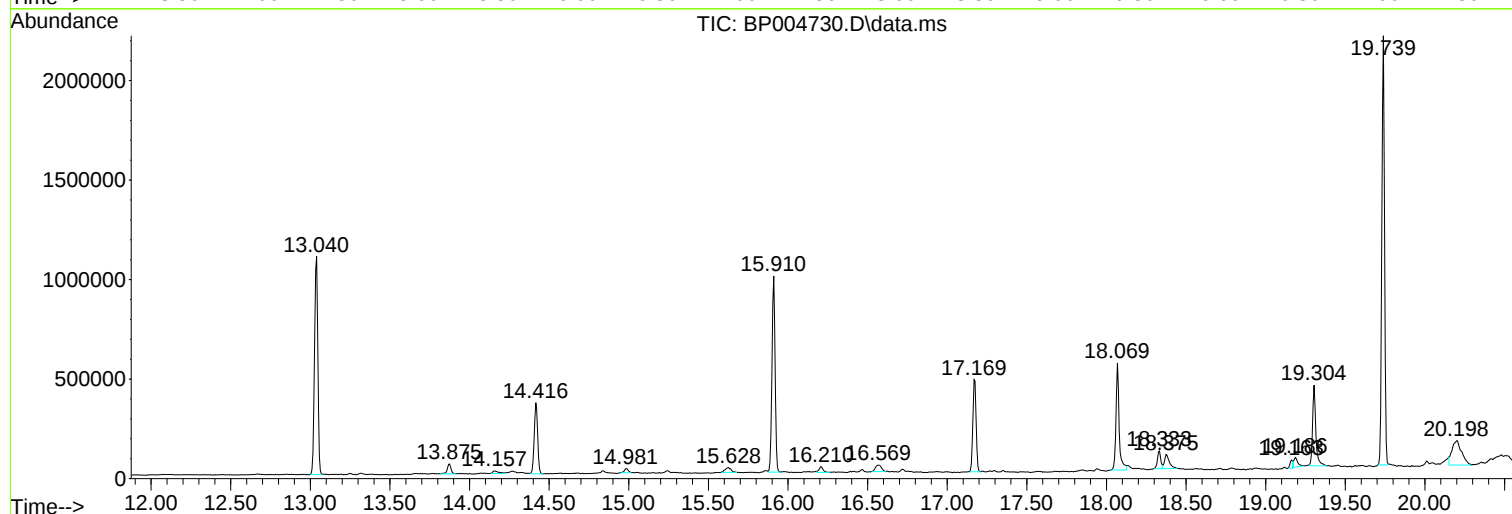
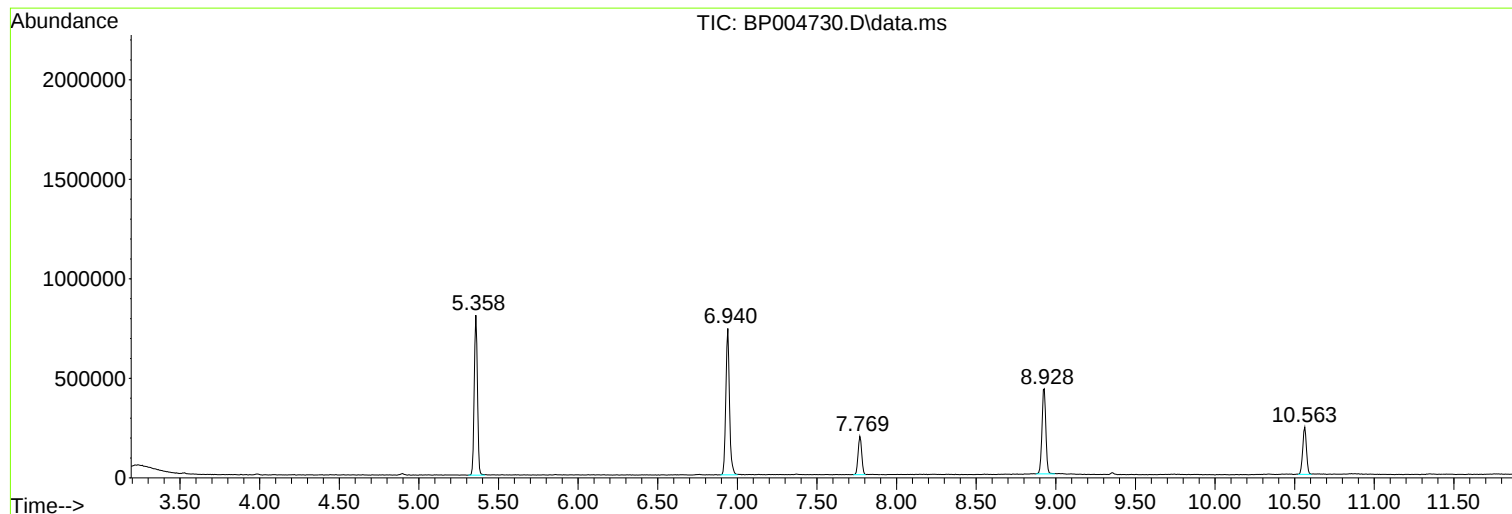
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BNA_P
ClientSampleId :
FK-BPM-04-013-ABCD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.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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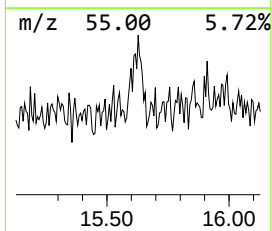
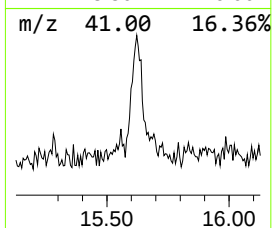
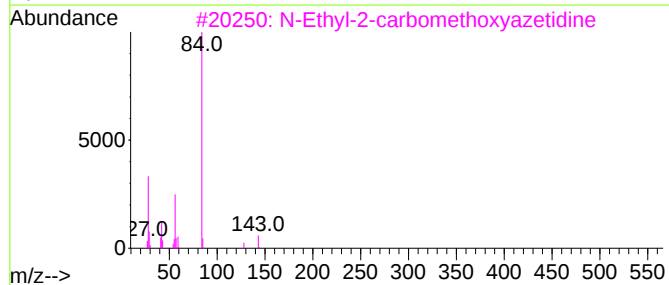
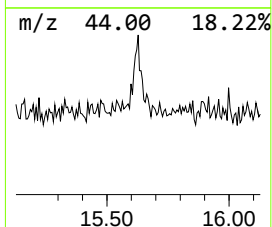
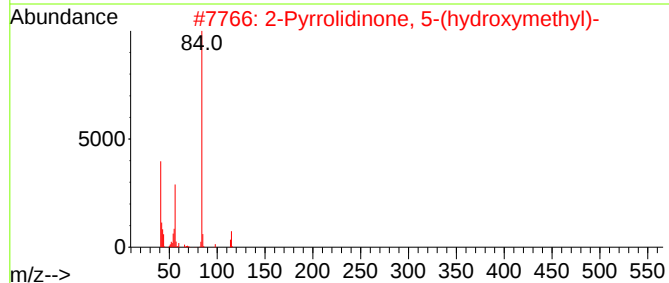
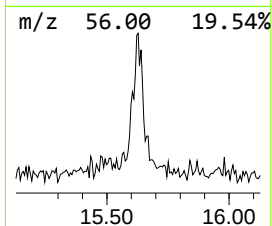
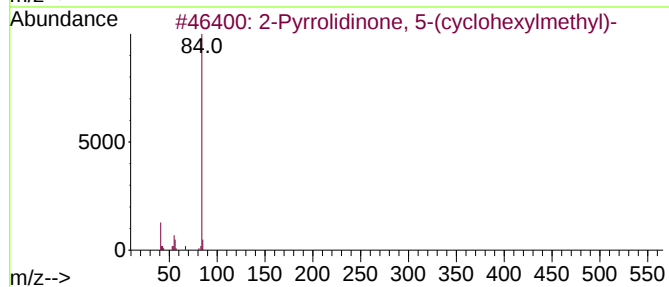
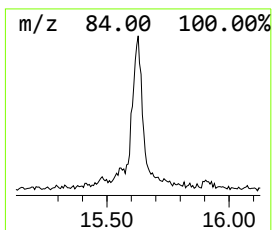
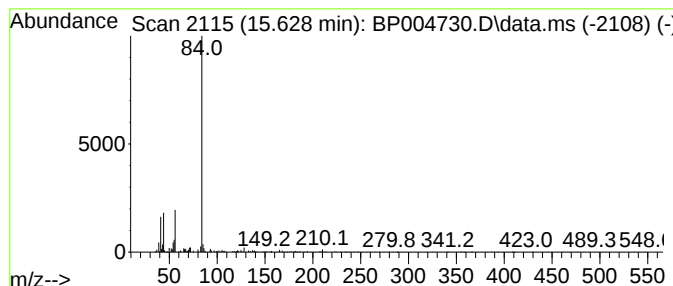
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown15.62 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.628	2.39 ng	63089	Acenaphthene-d10	14.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyrrolidinone, 5-(cyclohexylme...	181	C11H19NO	014293-08-4	40		
2	2-Pyrrolidinone, 5-(hydroxymethyl)-	115	C5H9NO2	062400-75-3	39		
3	N-Ethyl-2-carbomethoxyazetidine	143	C7H13NO2	054773-04-5	39		
4	1-Pyrrolid-2-one, N-carbamoyl-	128	C5H8N2O2	040451-67-0	38		
5	.gamma.-L-glutamyl-L-glutamic acid	276	C10H16N2O7	001116-22-9	38		



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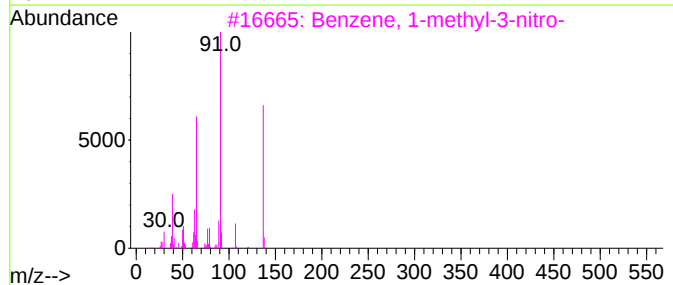
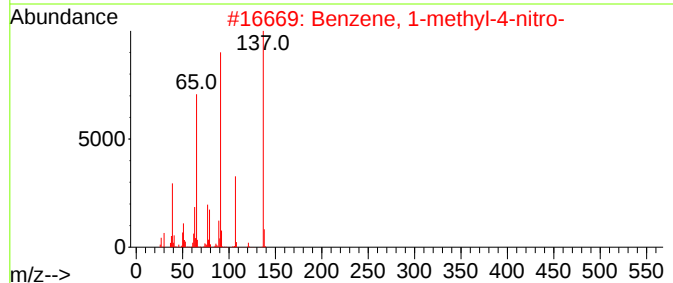
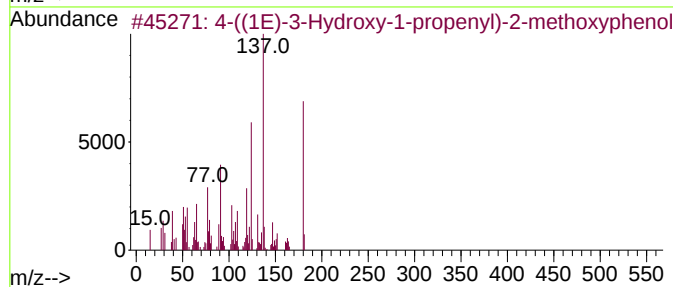
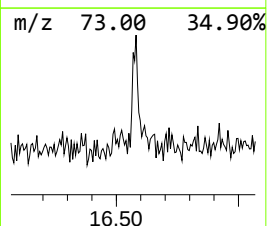
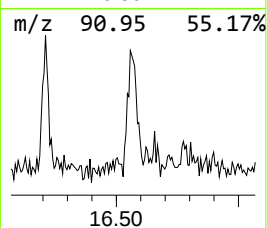
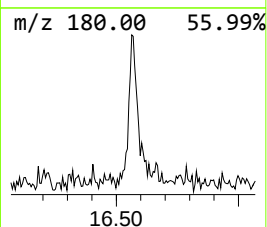
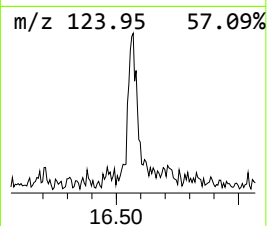
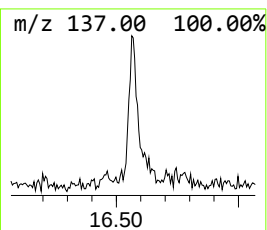
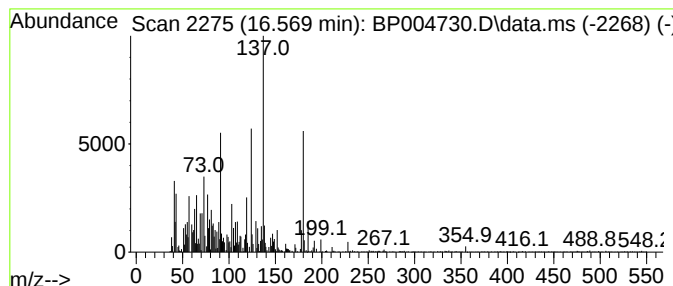
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.569	2.62 ng	84908	Phenanthrene-d10	17.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-((1E)-3-Hydroxy-1-propenyl)-2-methoxyphenol	180	C10H12O3	1000297-95-5	70
2			Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	46
3			Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	41
4			3,7-Benzofurandiol, 2,3-dihydro-	180	C10H12O3	017781-15-6	38
5			4-Fluorophenyl isocyanate	137	C7H4FNO	001195-45-5	38



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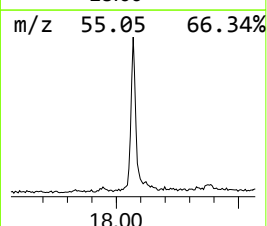
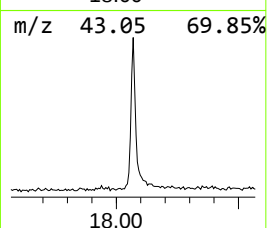
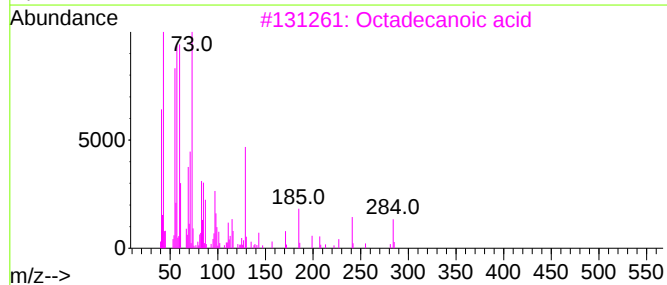
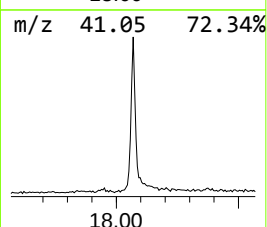
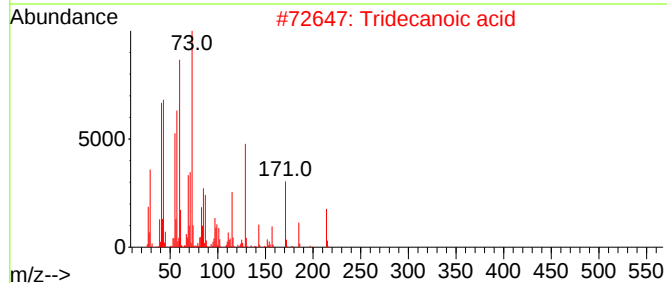
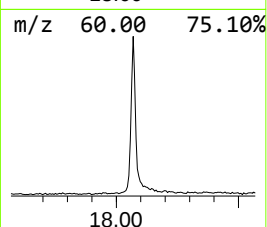
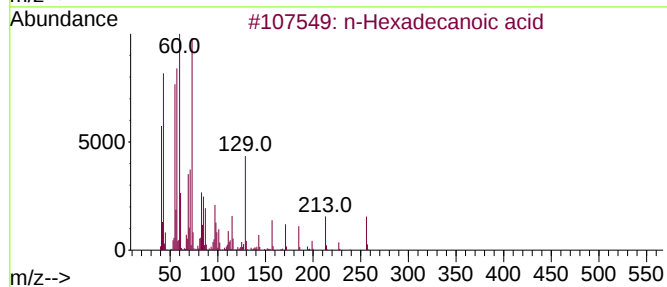
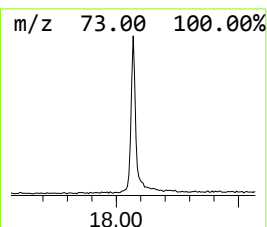
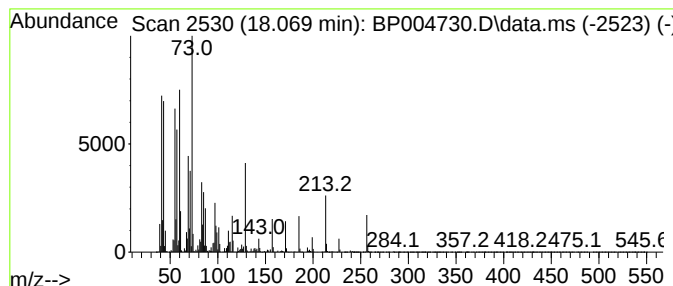
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.069	22.73 ng	737813	Phenanthrene-d10	17.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



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Misc :
ALS Vial : 5 Sample Multiplier: 1

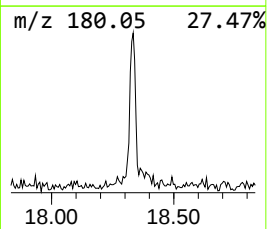
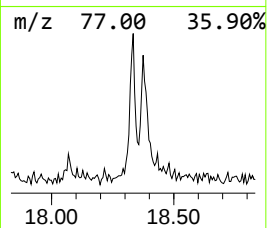
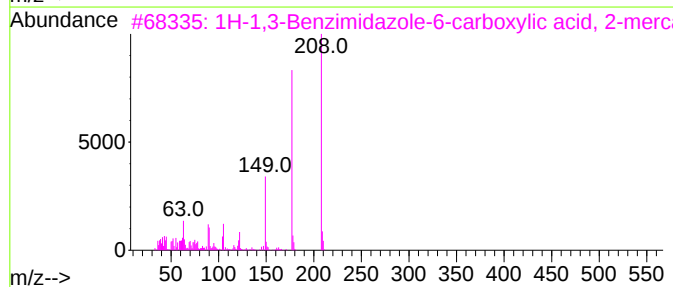
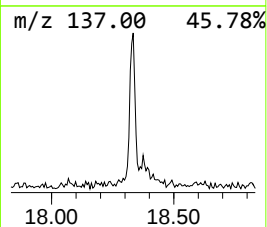
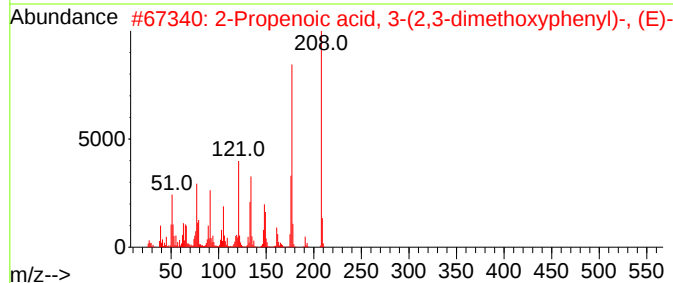
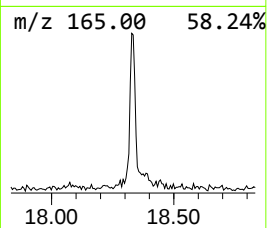
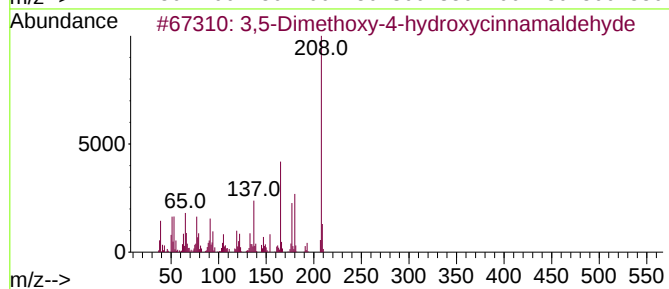
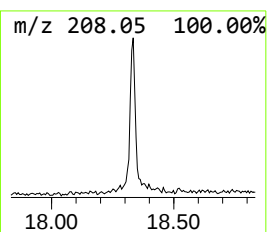
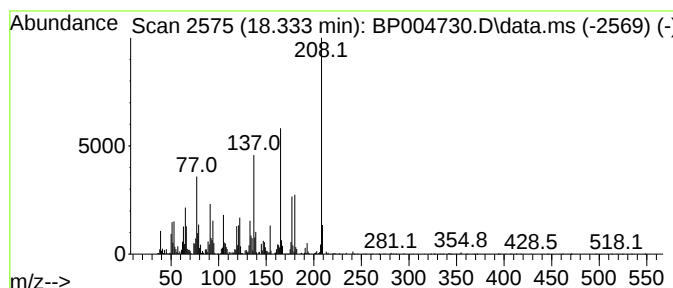
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.333	4.09 ng	132633	Phenanthrene-d10	17.169	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamal...	208	C11H12O4	087345-53-7	93
2	2-Propenoic acid, 3-(2,3-dimetho...	208	C11H12O4	007345-82-6	46
3	1H-1,3-Benzimidazole-6-carboxyli...	208	C9H8N2O2S	1000337-18-1	46
4	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	38
5	1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	38



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Misc :
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Instrument :
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ClientSampleId :
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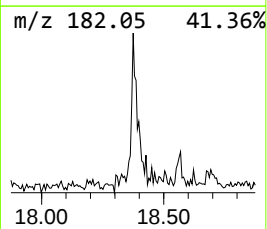
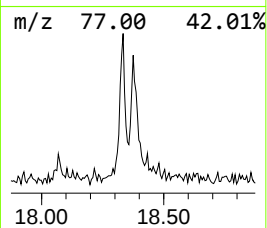
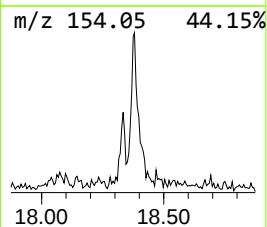
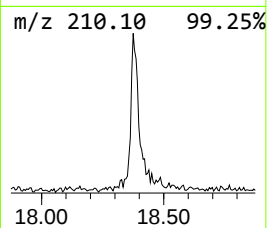
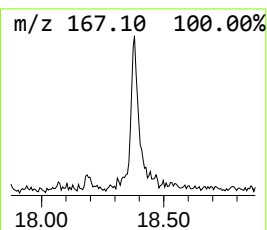
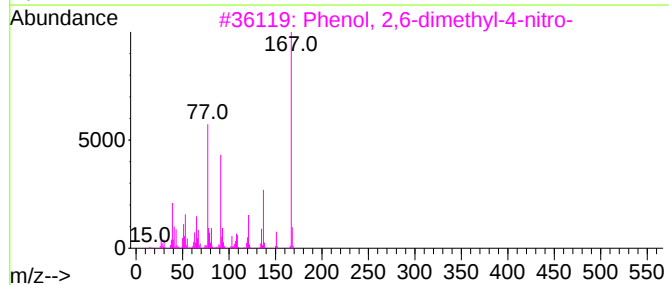
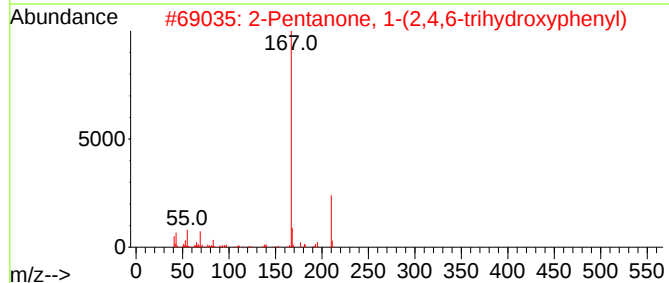
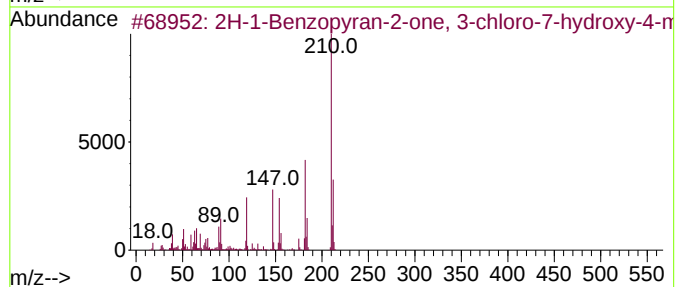
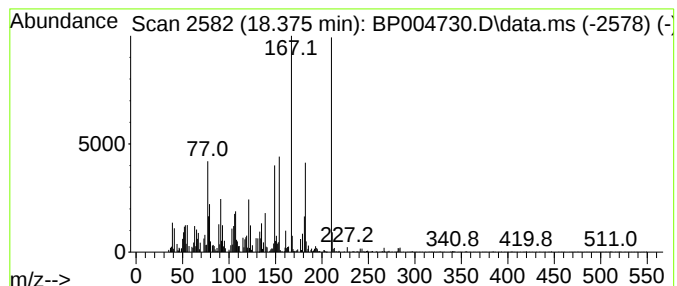
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown18.37 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.375	4.51 ng	146485	Phenanthrene-d10	17.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-1-Benzopyran-2-one, 3-chloro-...	210	C10H7ClO3	006174-86-3	41
2			2-Pentanone, 1-(2,4,6-trihydroxy...	210	C11H14O4	1000116-22-3	38
3			Phenol, 2,6-dimethyl-4-nitro-	167	C8H9NO3	002423-71-4	30
4			1-Hydroxy-6-methylphenazine	210	C13H10N2O	014031-08-4	25
5			3-Isopropyl-1-methyl-4-methylami...	182	C9H14N2O2	1000296-12-2	22



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Misc :
ALS Vial : 5 Sample Multiplier: 1

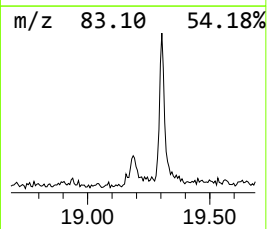
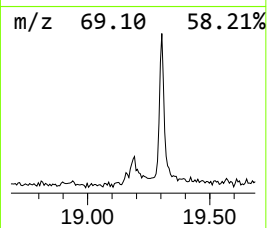
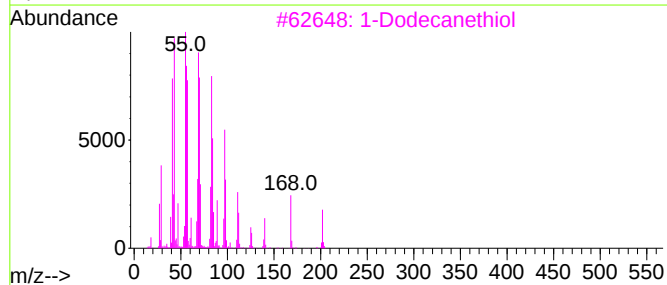
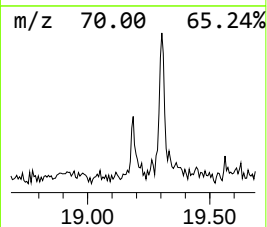
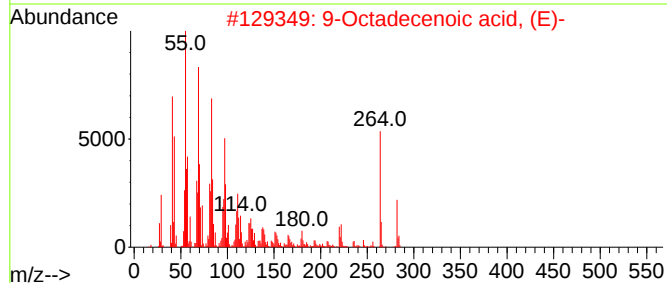
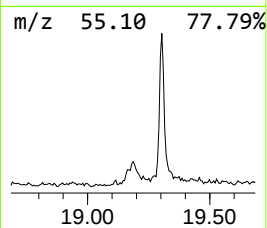
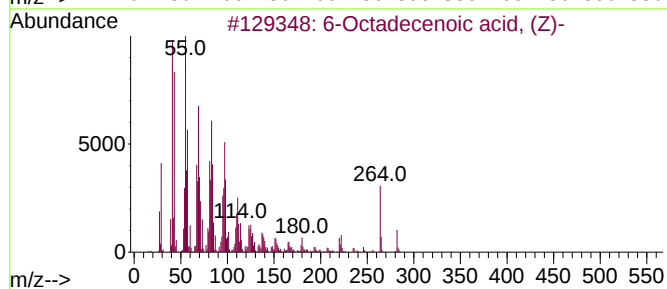
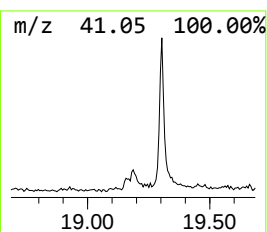
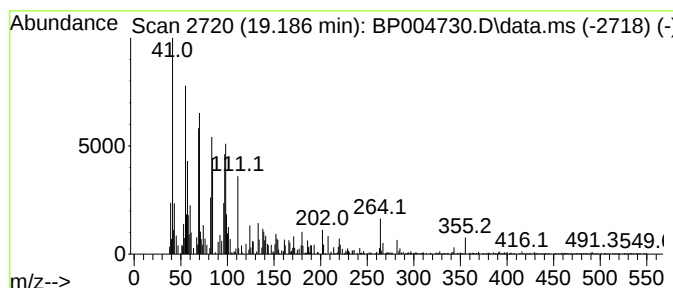
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 6-Octadecenoic acid, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.186	2.33 ng	75546	Phenanthrene-d10		17.169	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, (Z)-		282	C18H34O2	000593-39-5	70
2	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	64
3	1-Dodecanethiol		202	C12H26S	000112-55-0	62
4	2-Cyclohexen-1-ol		98	C6H10O	000822-67-3	43
5	Cycloheptane		98	C7H14	000291-64-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004730.D
Acq On : 12 Feb 2021 15:16
Operator : CG/JU
Sample : M1396-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FK-BPM-04-013-ABCD

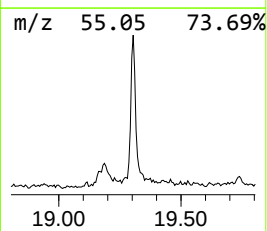
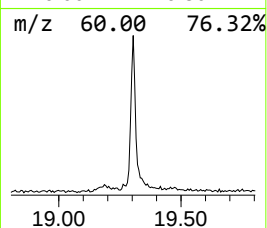
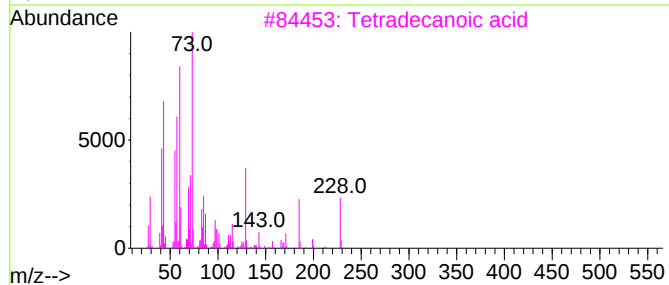
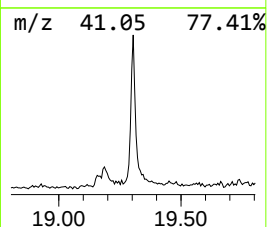
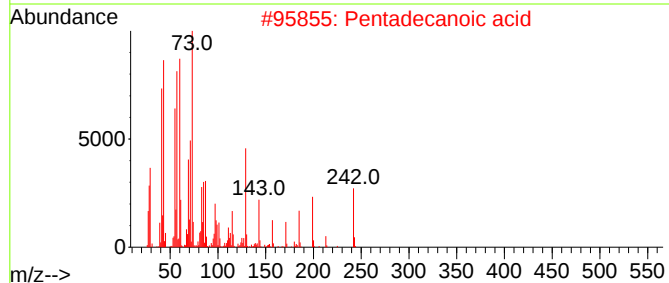
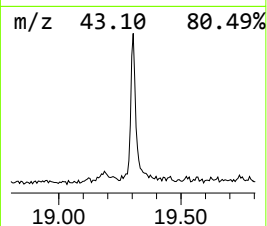
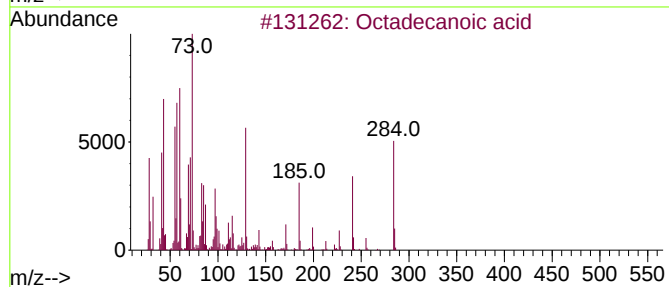
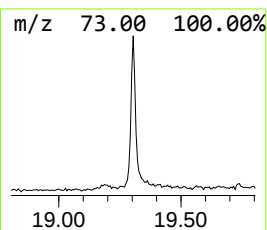
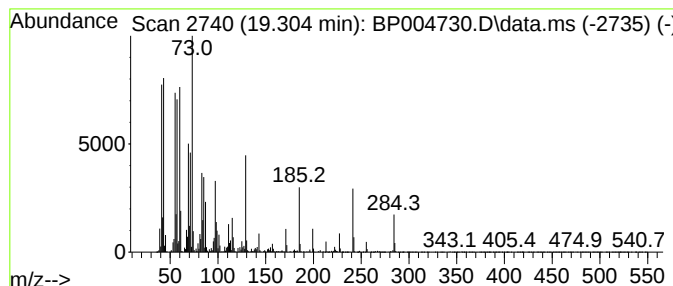
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.304	14.21 ng	560200	Chrysene-d12	21.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004730.D
Acq On : 12 Feb 2021 15:16
Operator : CG/JU
Sample : M1396-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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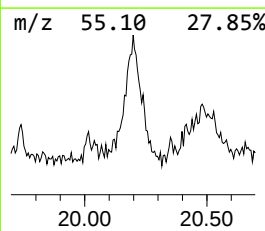
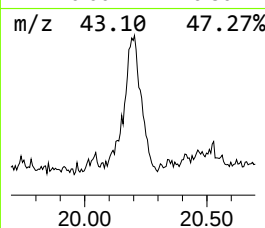
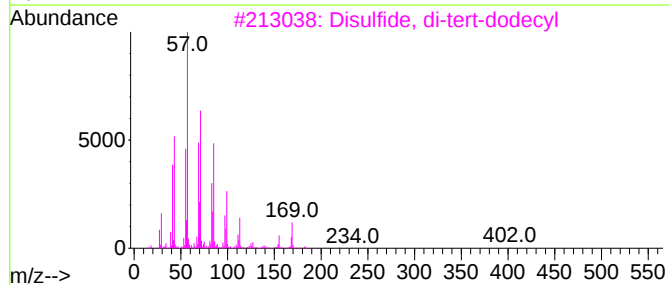
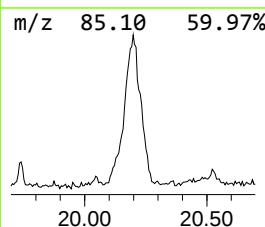
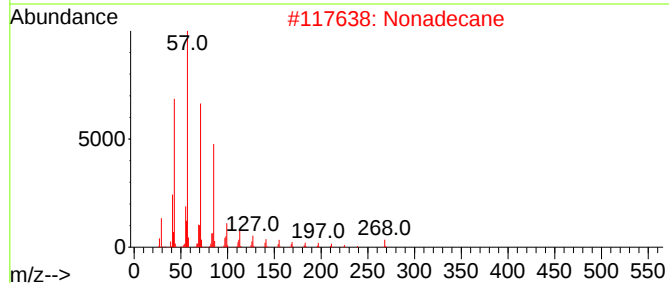
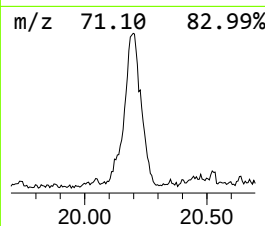
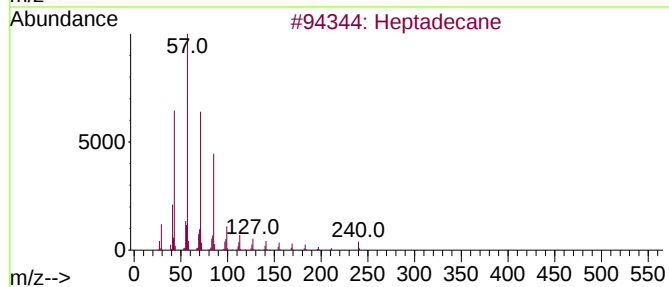
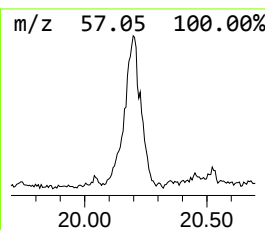
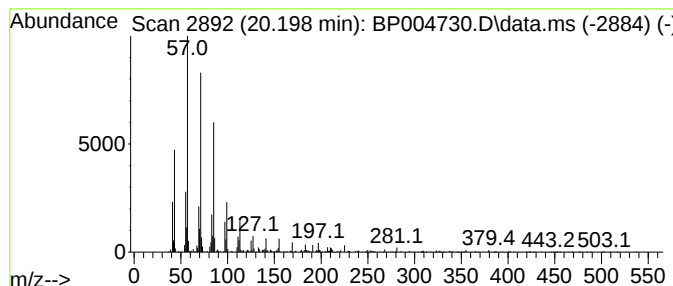
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.198	12.91 ng	508908	Chrysene-d12	21.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	95
2			Nonadecane	268	C19H40	000629-92-5	94
3			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	94
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
5			Octadecane	254	C18H38	000593-45-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004730.D
Acq On : 12 Feb 2021 15:16
Operator : CG/JU
Sample : M1396-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

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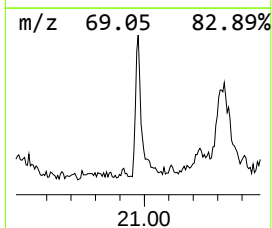
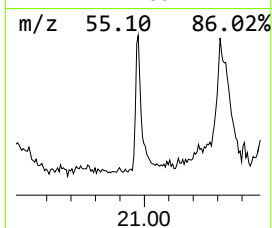
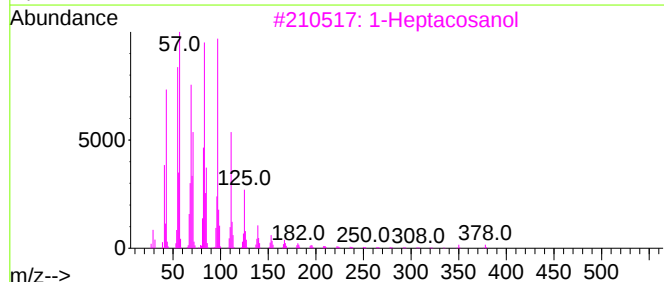
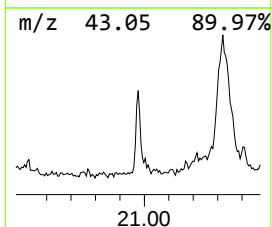
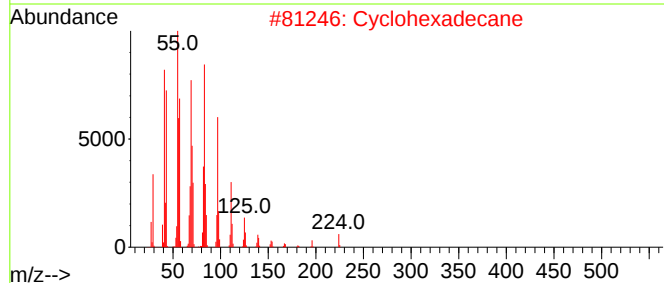
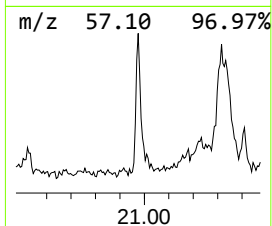
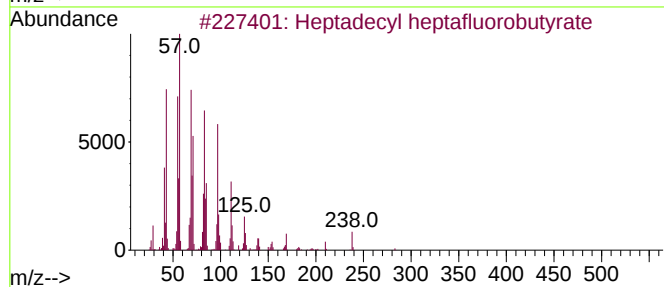
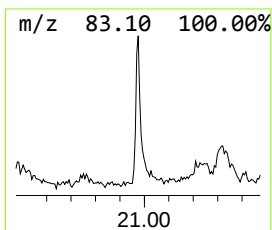
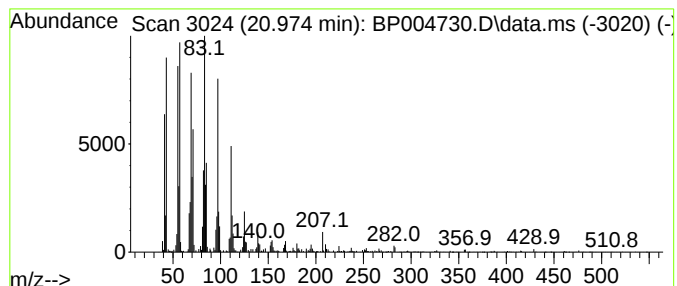
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	5.67 ng	223347	Chrysene-d12	21.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2			Cyclohexadecane	224	C16H32	000295-65-8	89
3			1-Heptacosanol	396	C27H56O	002004-39-9	87
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
5			Behenic alcohol	326	C22H46O	000661-19-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004730.D
Acq On : 12 Feb 2021 15:16
Operator : CG/JU
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ALS Vial : 5 Sample Multiplier: 1

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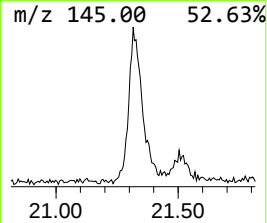
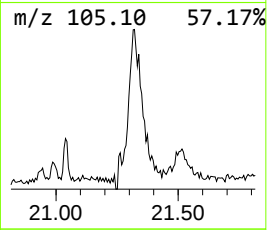
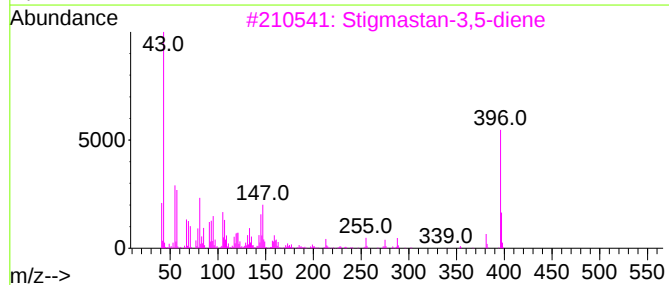
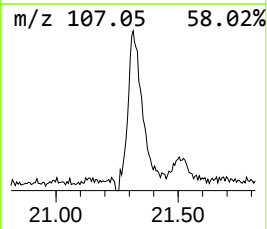
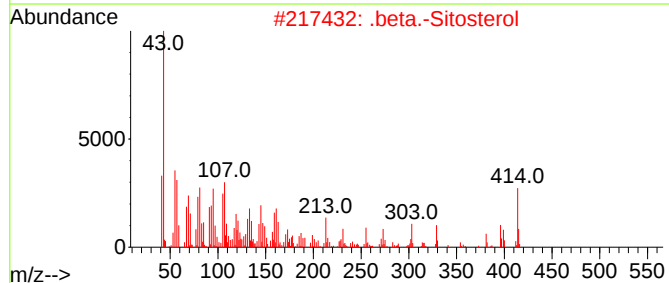
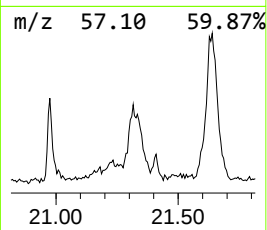
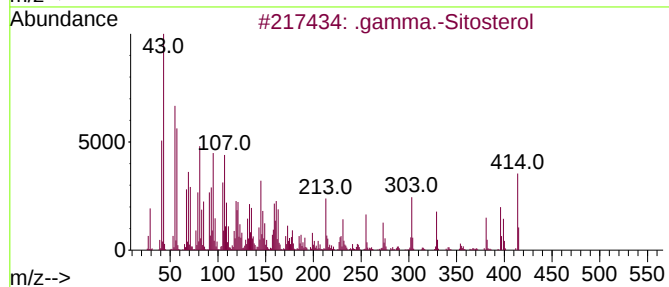
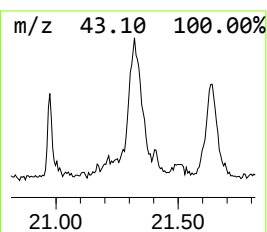
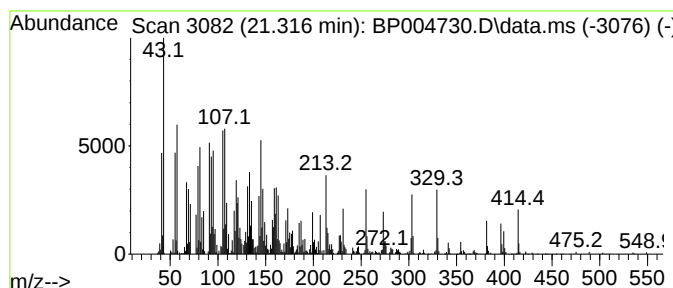
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.316	27.76 ng	1094330	Chrysene-d12	21.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2			.beta.-Sitosterol	414	C29H50O	000083-46-5	96
3			Stigmastan-3,5-diene	396	C29H48	1000214-16-4	35
4			Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	22
5			Stigmastan-3-en-6-ol	414	C29H50O	1000214-19-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004730.D
Acq On : 12 Feb 2021 15:16
Operator : CG/JU
Sample : M1396-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
FK-BPM-04-013-ABCD

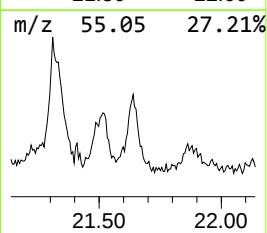
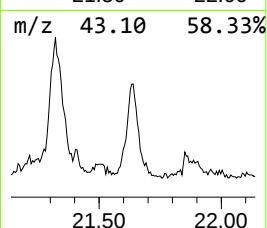
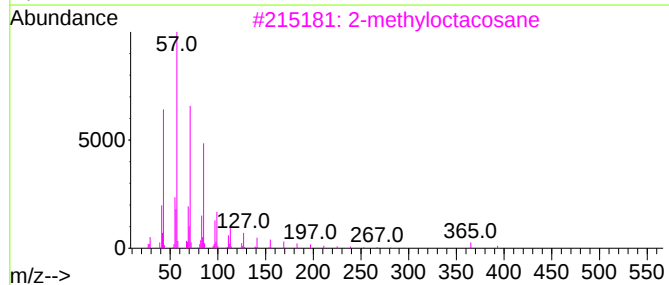
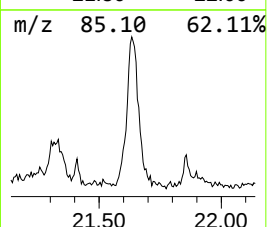
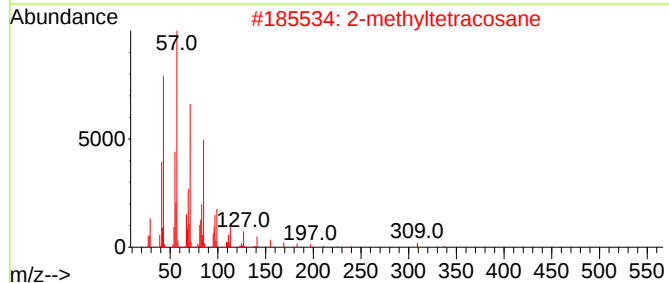
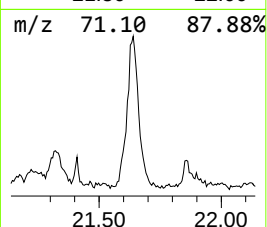
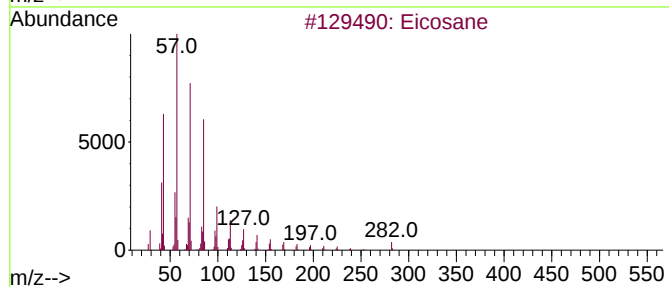
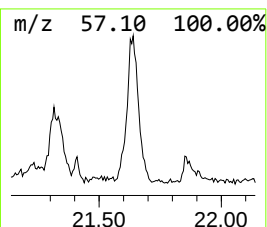
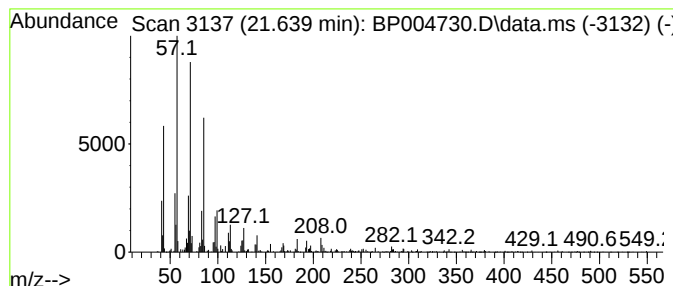
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.639	9.21 ng	363265	Chrysene-d12	21.257

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			2-methyltetracosane	352	C25H52	1000376-72-6	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021221\
Data File : BP004730.D
Acq On : 12 Feb 2021 15:16
Operator : CG/JU
Sample : M1396-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
FK-BPM-04-013-ABCD

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020521.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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					#	RT	Resp	Conc
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4-((1E)-3-Hydro...	16.569	2.6	ng	84908	4	17.169	649150	20.0
n-Hexadecanoic ...	18.069	22.7	ng	737813	4	17.169	649150	20.0
3,5-Dimethoxy-4...	18.333	4.1	ng	132633	4	17.169	649150	20.0
unknown18.37	18.375	4.5	ng	146485	4	17.169	649150	20.0
6-Octadecenoic ...	19.186	2.3	ng	75546	4	17.169	649150	20.0
Octadecanoic acid	19.304	14.2	ng	560200	5	21.257	788467	20.0
Heptadecane	20.198	12.9	ng	508908	5	21.257	788467	20.0
Heptadecyl hept...	20.974	5.7	ng	223347	5	21.257	788467	20.0
.gamma.-Sitosterol	21.316	27.8	ng	1094330	5	21.257	788467	20.0
Eicosane	21.639	9.2	ng	363265	5	21.257	788467	20.0