

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
 Data File : BP005400.D
 Acq On : 23 Apr 2021 18:48
 Operator : CG/JU
 Sample : M2149-16
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-40-9.5-10.0-DUP

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-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005400.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	358	365	377	rBV	705774	1008447	47.38%	9.270%
2	6.822	626	635	650	rBV	647640	1062250	49.91%	9.765%
3	7.634	766	773	781	rBV	111487	171794	8.07%	1.579%
4	8.799	962	971	984	rBV	402995	663983	31.19%	6.104%
5	10.422	1240	1247	1254	rBV	119107	197740	9.29%	1.818%
6	12.910	1662	1670	1682	rBV	790341	1131776	53.17%	10.404%
7	13.763	1810	1815	1825	rBV	16415	30769	1.45%	0.283%
8	14.298	1900	1906	1915	rVB2	167509	246261	11.57%	2.264%
9	15.804	2155	2162	2173	rBV	842876	1177281	55.31%	10.822%
10	17.069	2370	2377	2386	rBV	220985	323356	15.19%	2.973%
11	17.975	2525	2531	2539	rBV	107885	166567	7.83%	1.531%
12	19.210	2737	2741	2748	rBV	57182	85940	4.04%	0.790%
13	19.475	2776	2786	2796	rBV	20525	73525	3.45%	0.676%
14	19.651	2810	2816	2824	rVB	1897801	2128507	100.00%	19.567%
15	19.922	2859	2862	2865	rBV3	23673	32155	1.51%	0.296%
16	20.604	2975	2978	2983	rBV2	26910	30085	1.41%	0.277%
17	20.857	3016	3021	3022	rBV2	20496	29605	1.39%	0.272%
18	20.886	3022	3026	3034	rVV2	290062	421022	19.78%	3.870%
19	20.957	3035	3038	3046	rVB	62004	85253	4.01%	0.784%
20	21.175	3070	3075	3085	rBV	400231	495851	23.30%	4.558%
21	21.498	3126	3130	3135	rBV2	82014	91948	4.32%	0.845%
22	21.775	3172	3177	3187	rVB	214277	352499	16.56%	3.240%
23	22.451	3288	3292	3297	rVB2	84891	122092	5.74%	1.122%
24	22.786	3345	3349	3359	rVB6	65132	119339	5.61%	1.097%
25	23.433	3453	3459	3465	rBV2	264565	472315	22.19%	4.342%
26	23.863	3528	3532	3542	rVB2	73843	157771	7.41%	1.450%

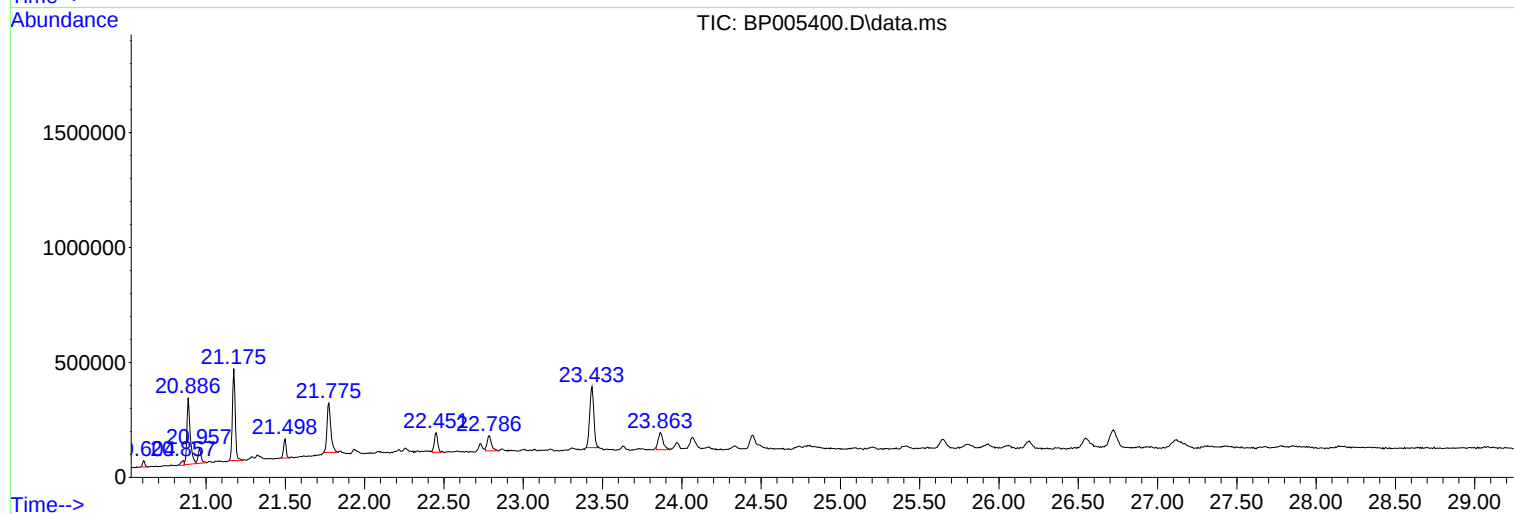
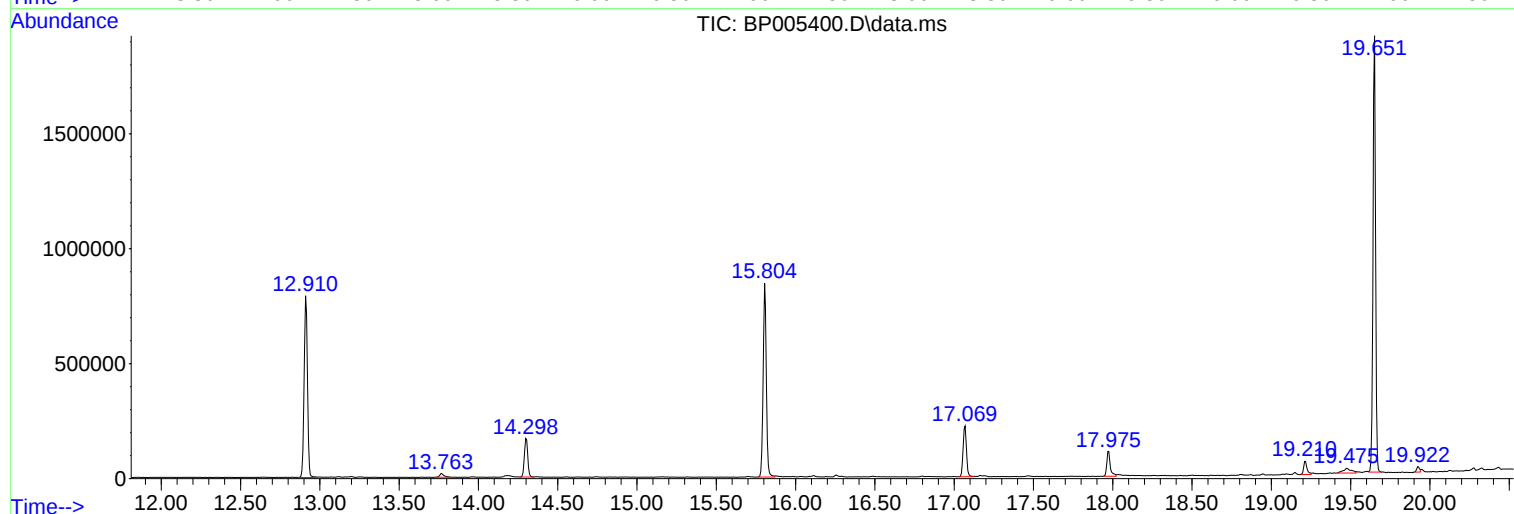
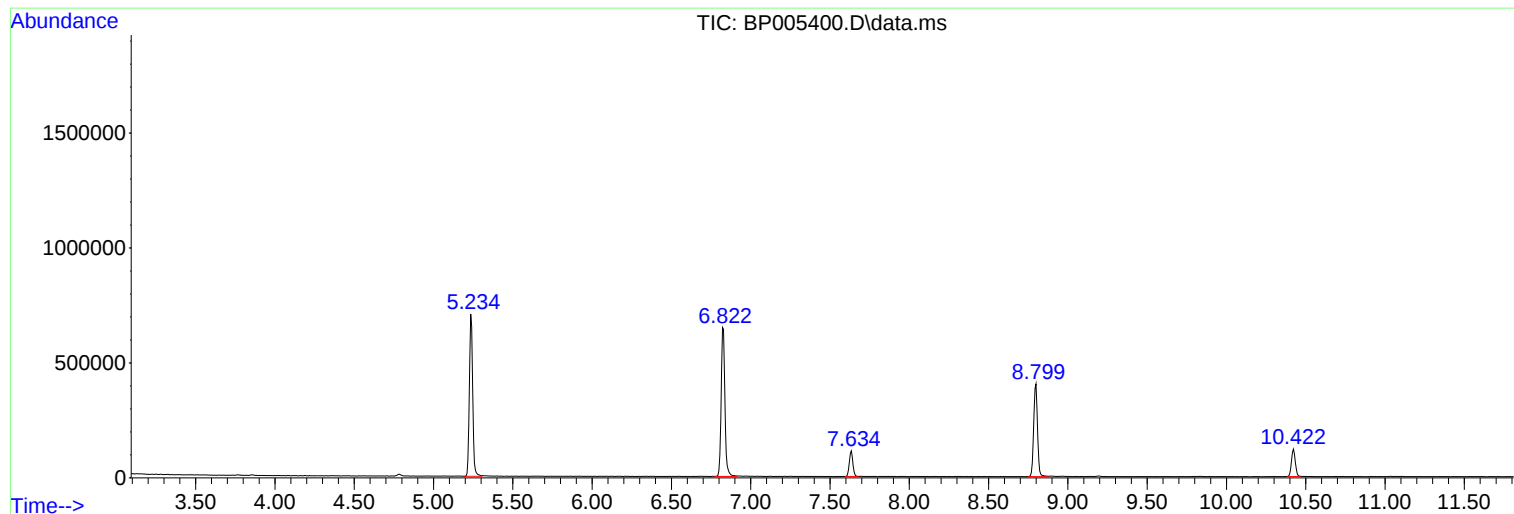
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-40-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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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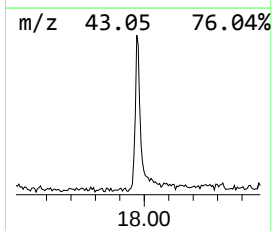
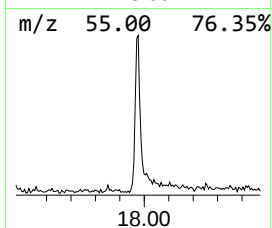
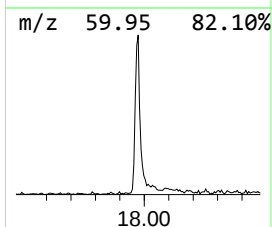
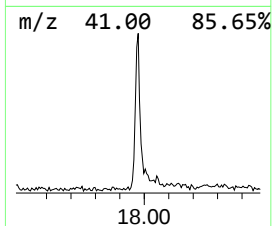
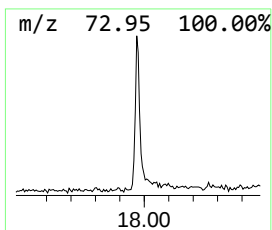
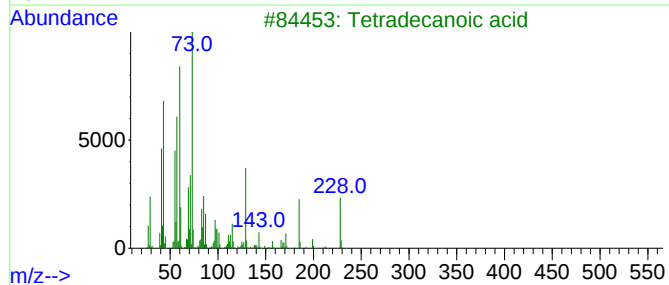
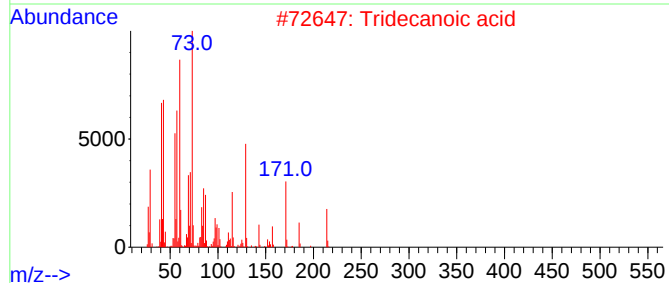
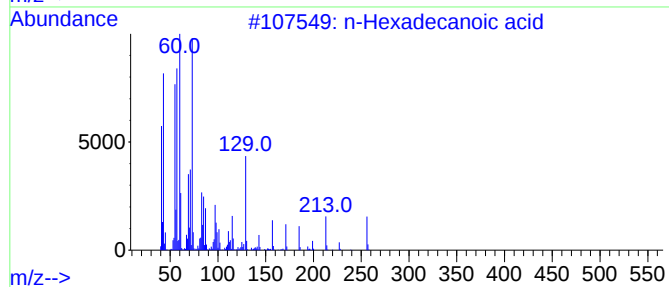
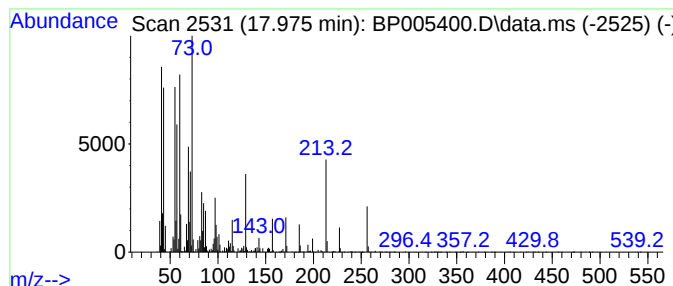
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.975	10.30 ng	166567	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid	284	C18H36O2	000057-11-4	58
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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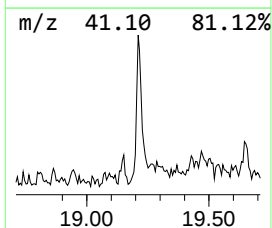
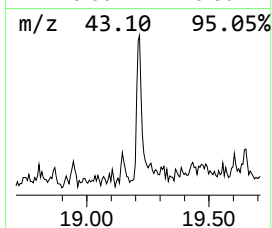
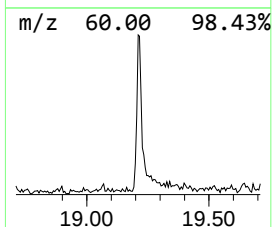
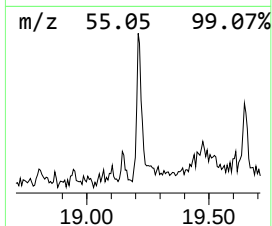
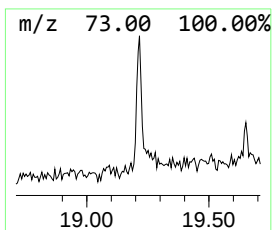
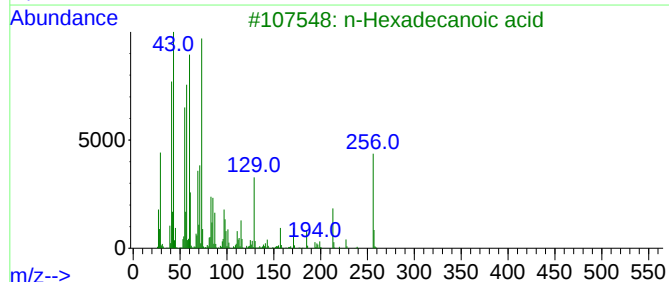
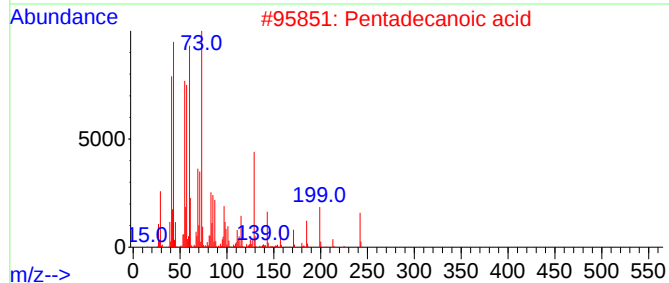
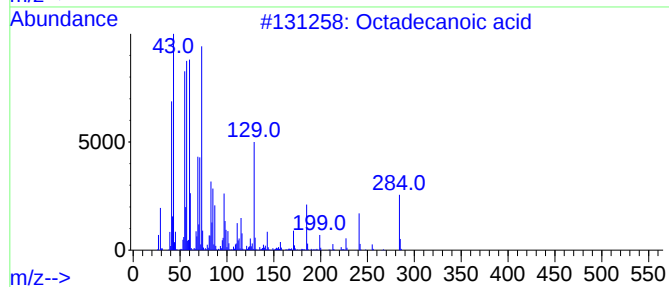
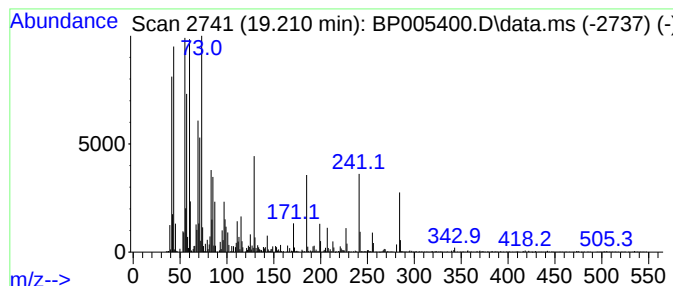
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.210	3.47 ng	85940	Chrysene-d12	21.175

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	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	86
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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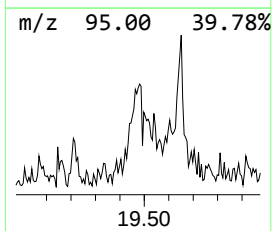
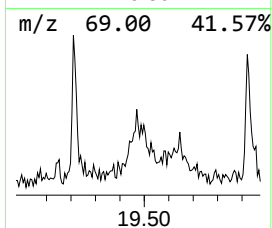
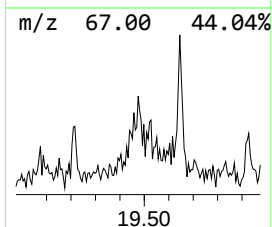
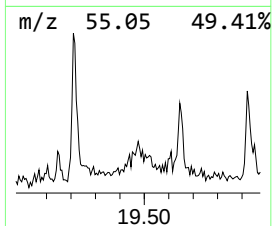
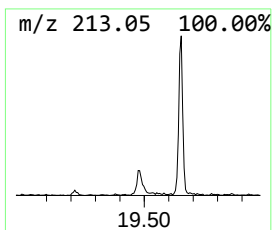
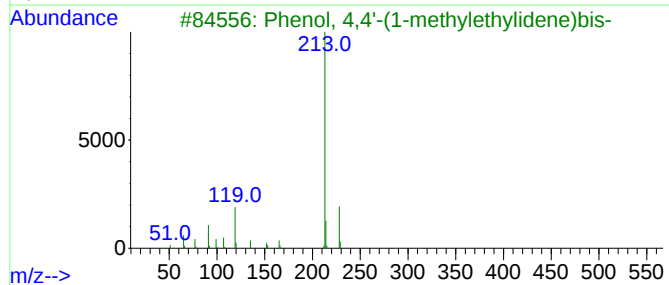
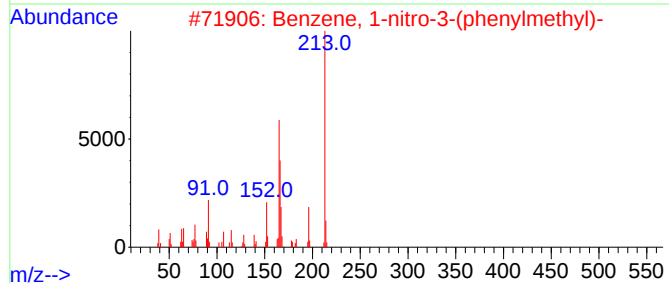
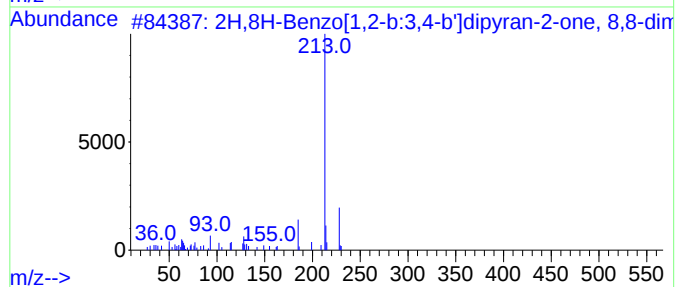
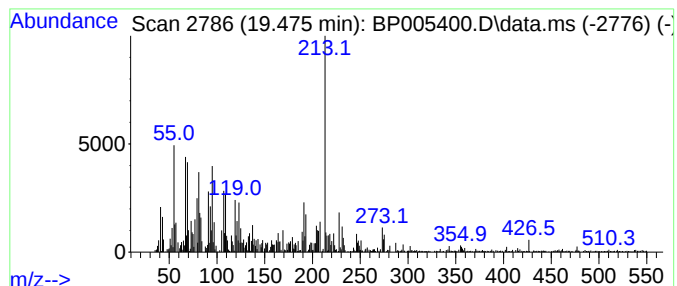
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown19.475 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.475	2.97 ng	73525	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	43
2			Benzene, 1-nitro-3-(phenylmethyl)-	213	C13H11NO2	005840-41-5	43
3			Phenol, 4,4'-(1-methylethylidene)...	228	C15H16O2	000080-05-7	43
4			Sebacic acid, ethyl 2,3,5,6-tetr...	442	C18H22C14O4	1000355-28-8	43
5			Benzoic acid, 2-(4-aminophenyl)-	213	C13H11NO2	025829-61-2	38



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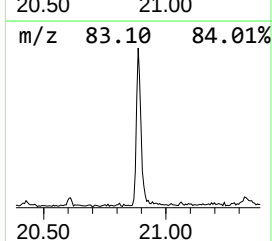
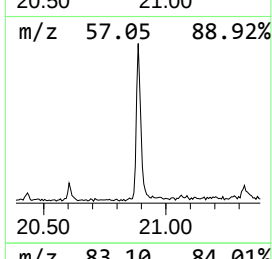
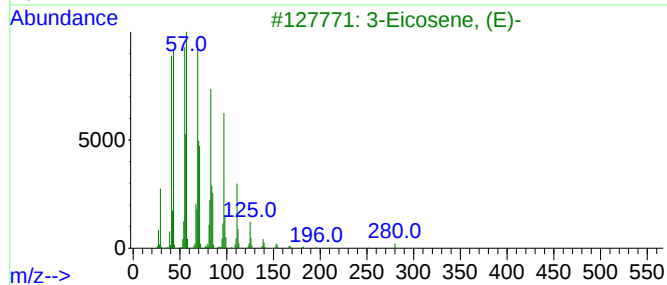
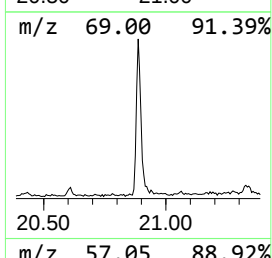
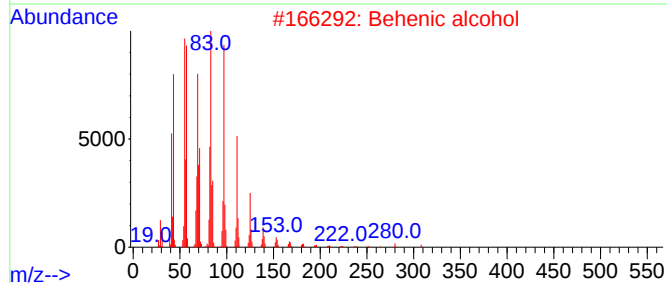
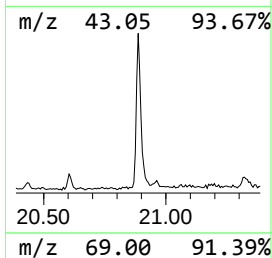
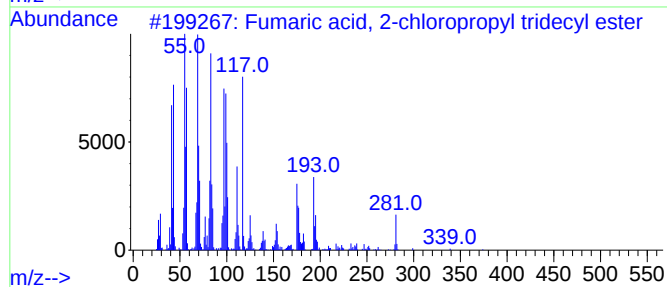
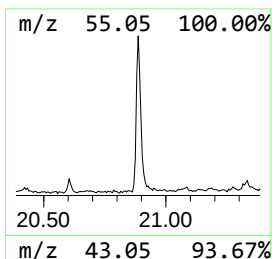
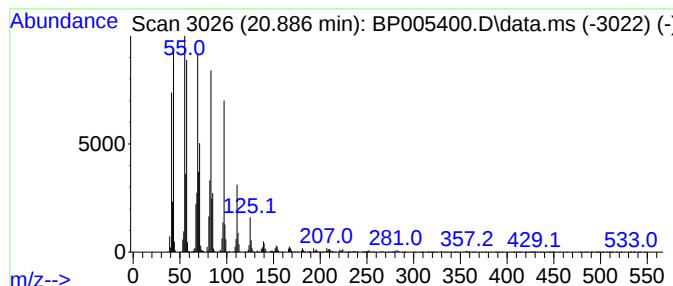
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Peak Number 4 Fumaric acid, 2-chloropropyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	16.98 ng	421022	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	98
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4			n-Pentadecanol	228	C15H32O	000629-76-5	91
5			1-Hexadecanol	242	C16H34O	036653-82-4	90



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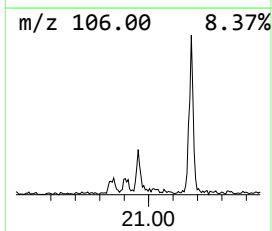
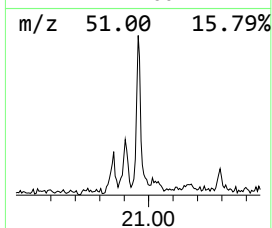
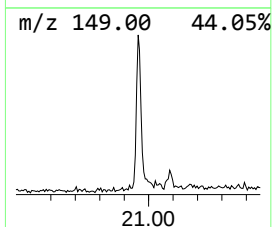
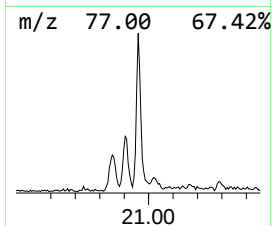
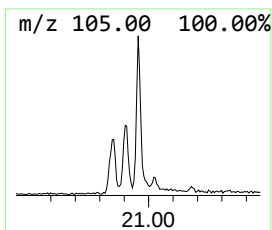
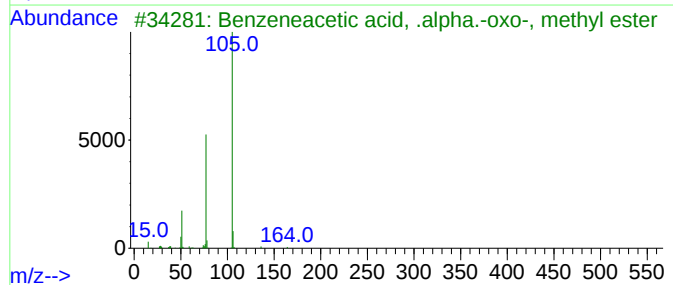
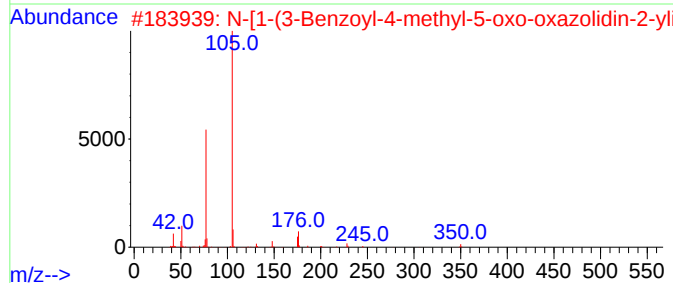
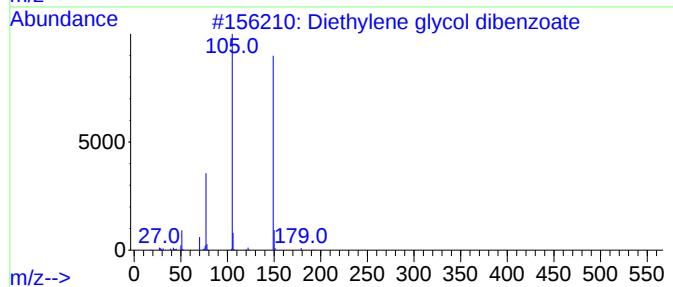
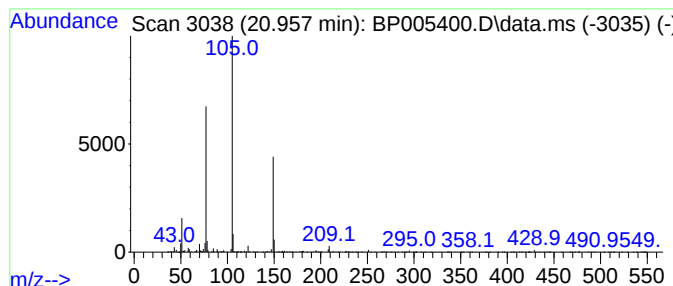
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.44 ng	85253	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	64
2			N-[1-(3-Benzoyl-4-methyl-5-oxo-o...	350	C20H18N2O4	1000296-93-4	38
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	38
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	38
5			1,3,4-Oxadiazin-6-one, 5-isoprop...	216	C12H12N2O2	173973-78-9	38



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SB-40-9.5-10.0-DUP

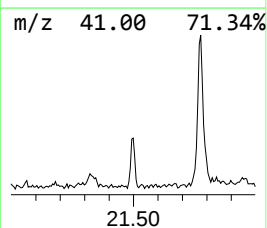
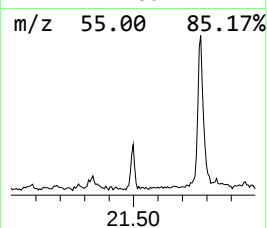
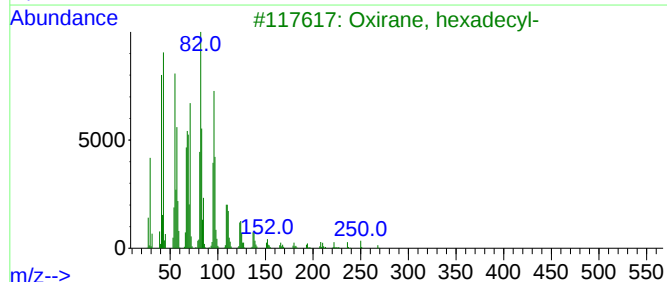
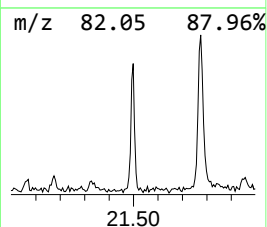
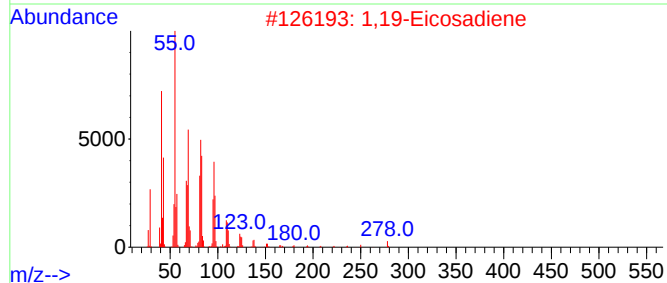
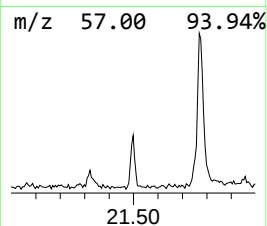
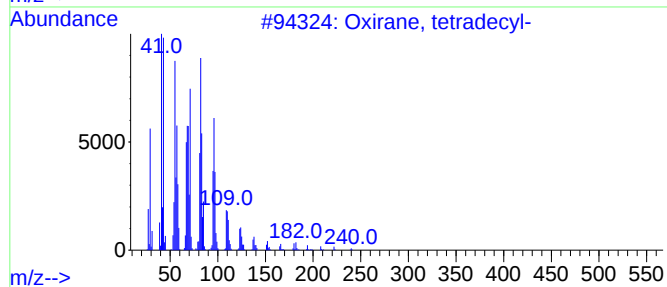
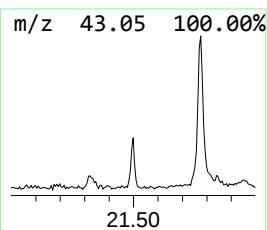
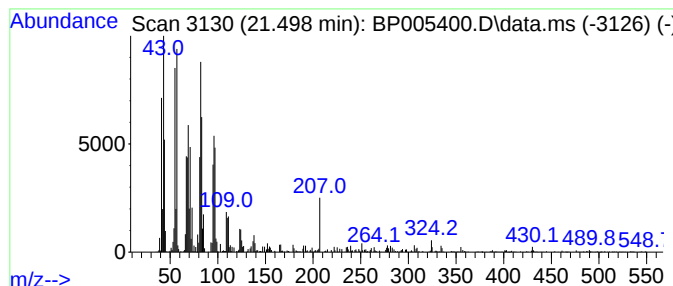
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, tetradecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.498	3.71 ng	91948	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, tetradecyl-	240	C16H32O	007320-37-8	96
2			1,19-Eicosadiene	278	C20H38	014811-95-1	90
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4			Octadecanal	268	C18H36O	000638-66-4	87
5			Z-11-Tetradecen-1-ol trifluoroac...	308	C16H27F3O2	1000131-33-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005400.D
Acq On : 23 Apr 2021 18:48
Operator : CG/JU
Sample : M2149-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-40-9.5-10.0-DUP

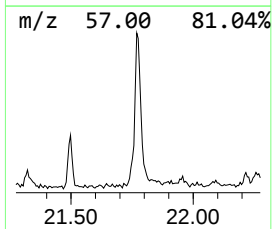
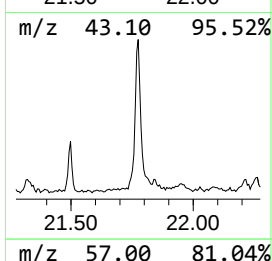
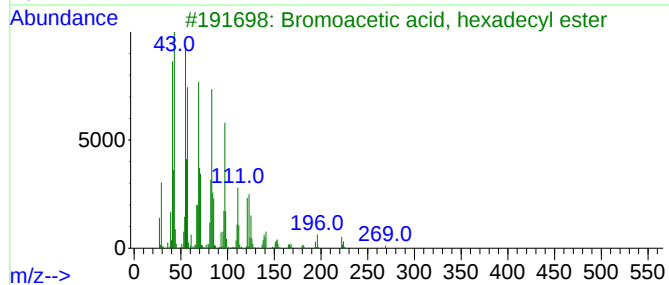
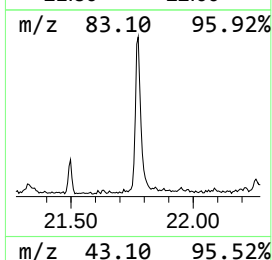
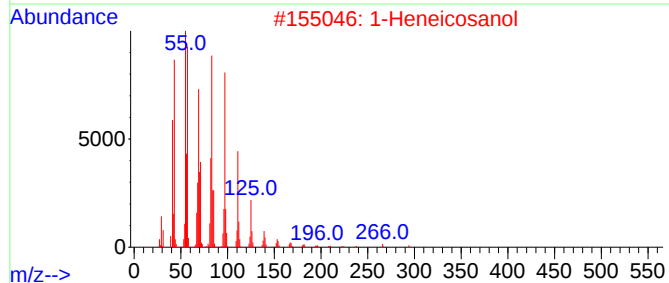
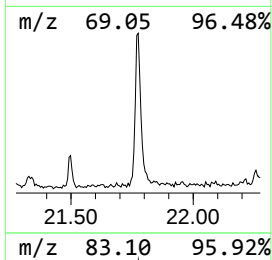
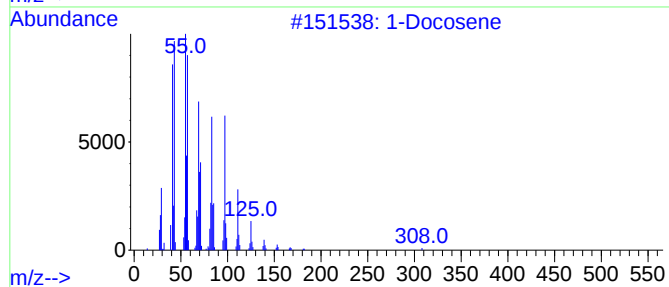
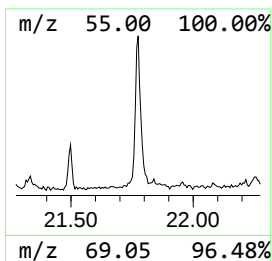
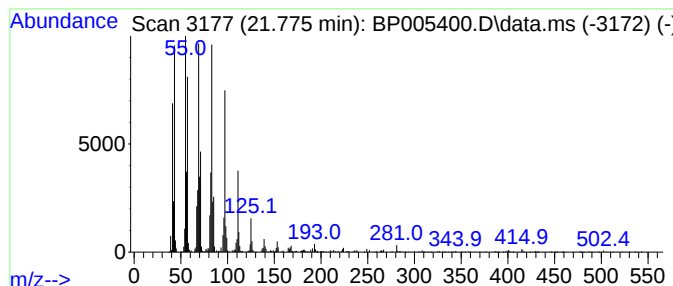
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.775	14.22 ng	352499	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	97
2	1-Heneicosanol			312	C21H44O	015594-90-8	91
3	Bromoacetic acid, hexadecyl ester			362	C18H35BrO2	005454-48-8	90
4	1-Heptacosanol			396	C27H56O	002004-39-9	89
5	n-Tetracosanol-1			354	C24H50O	000506-51-4	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005400.D
Acq On : 23 Apr 2021 18:48
Operator : CG/JU
Sample : M2149-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-40-9.5-10.0-DUP

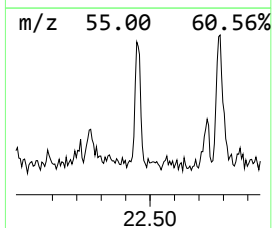
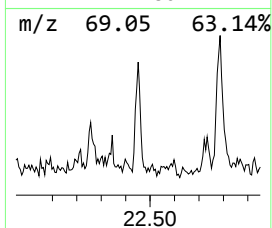
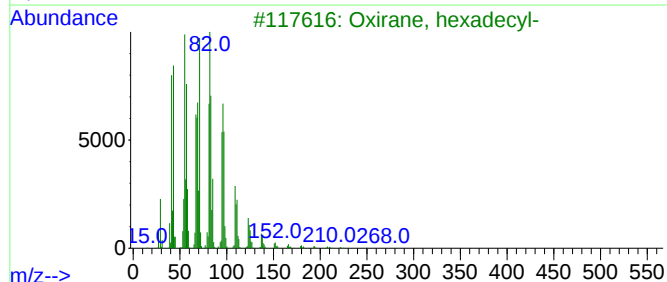
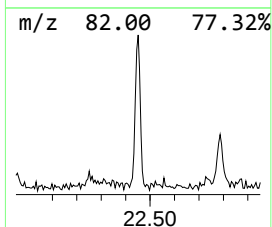
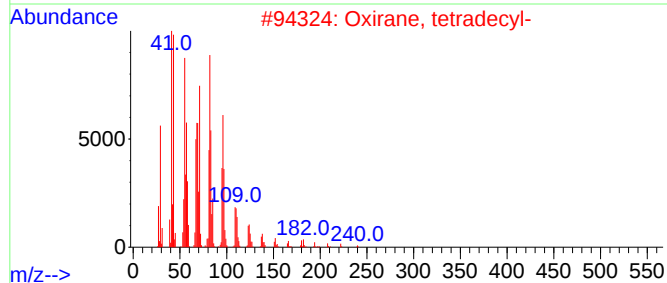
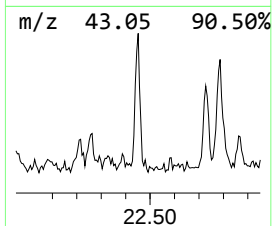
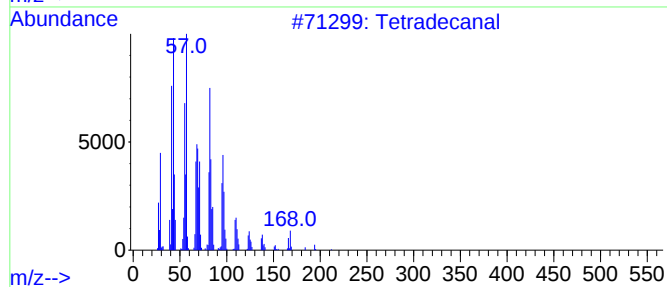
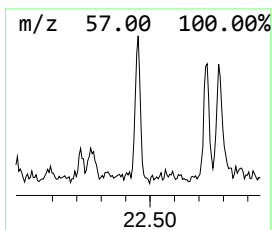
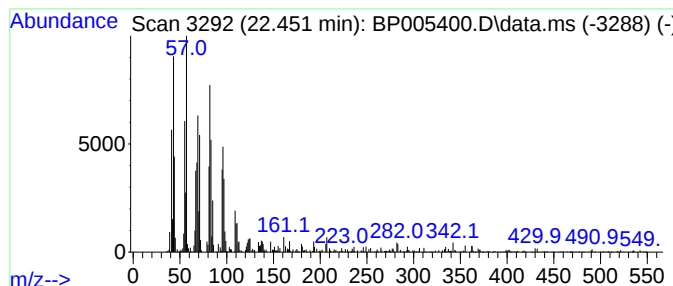
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetradecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.451	5.17 ng	122092	Perylene-d12	23.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanal	212	C14H28O	000124-25-4	94
2			Oxirane, tetradecyl-	240	C16H32O	007320-37-8	94
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
4			Octadecanal	268	C18H36O	000638-66-4	87
5			1,19-Eicosadiene	278	C20H38	014811-95-1	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005400.D
Acq On : 23 Apr 2021 18:48
Operator : CG/JU
Sample : M2149-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-40-9.5-10.0-DUP

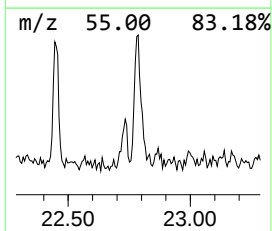
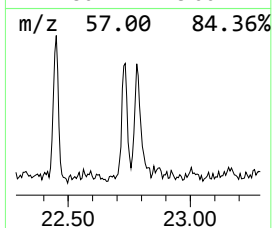
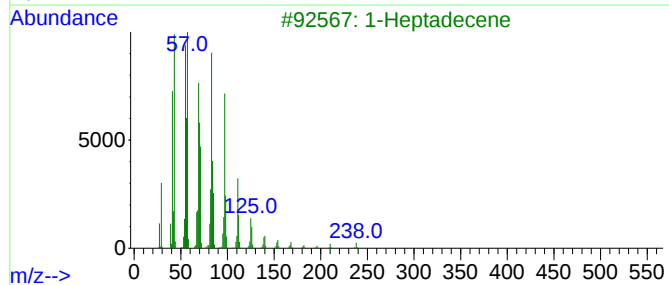
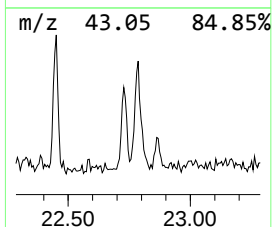
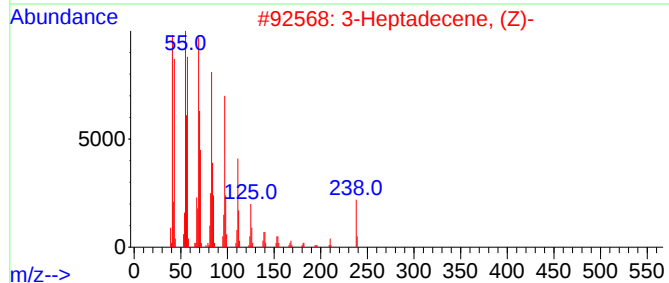
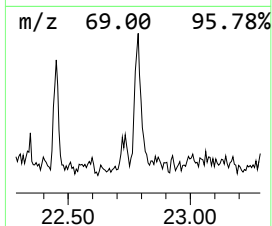
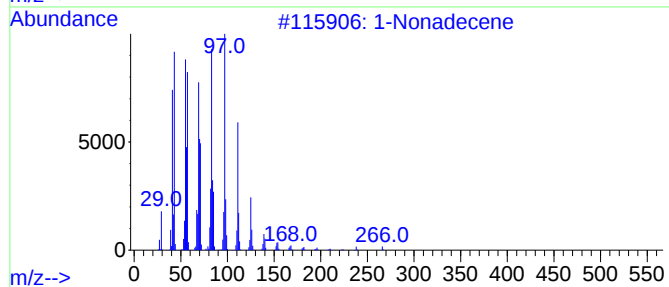
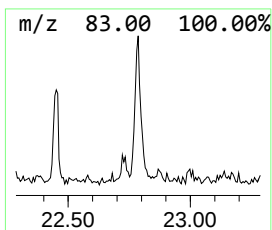
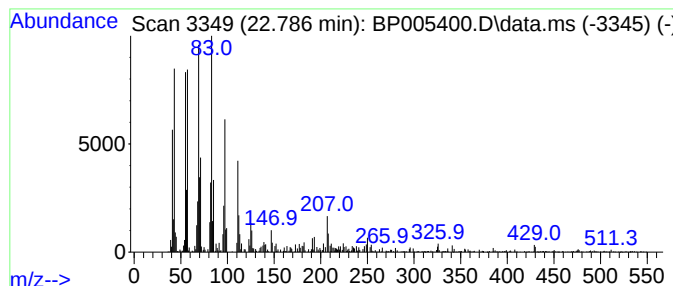
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.786	5.05 ng	119339	Perylene-d12	23.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	86
2	3-Heptadecene, (Z)-			238	C17H34	1000141-67-3	83
3	1-Heptadecene			238	C17H34	006765-39-5	81
4	1-Hexacosanol			382	C26H54O	000506-52-5	70
5	Cetene			224	C16H32	000629-73-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005400.D
Acq On : 23 Apr 2021 18:48
Operator : CG/JU
Sample : M2149-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-40-9.5-10.0-DUP

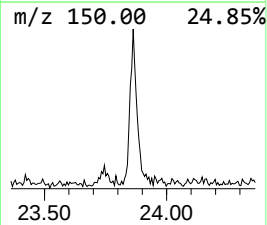
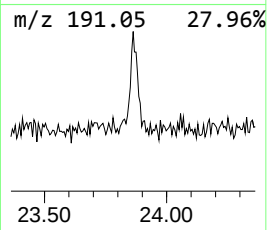
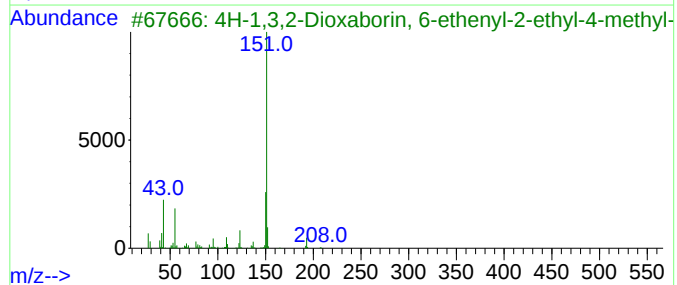
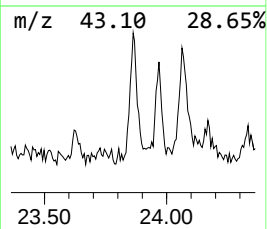
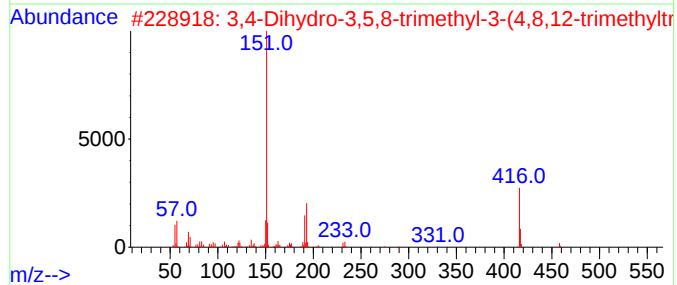
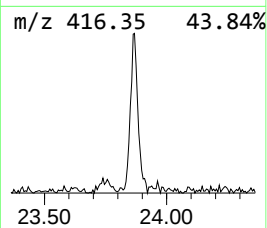
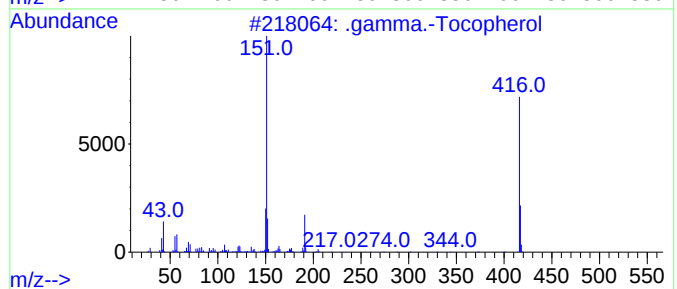
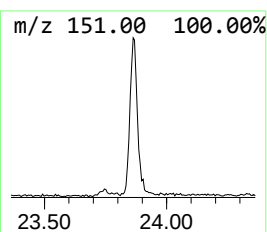
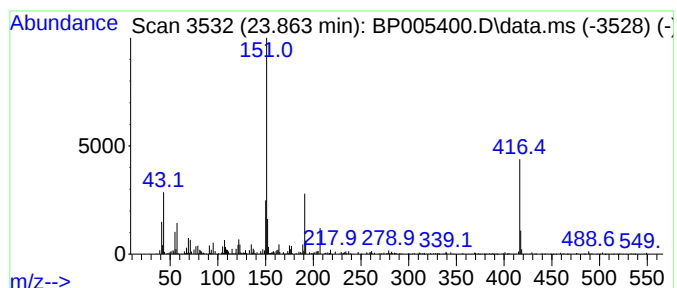
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Tocopherol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.863	6.68 ng	157771	Perylene-d12	23.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Tocopherol	416	C28H48O2	007616-22-0	94
2			3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	58
3			4H-1,3,2-Dioxaborin, 6-ethenyl-2...	208	C12H21BO2	074630-05-0	37
4			Dimethyl-(allyl)-silyloxybenzene	192	C11H16OSi	066998-68-3	30
5			Dichloromethyldimethylsilyloxybe...	234	C9H12Cl2OSi	1000299-10-7	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
Data File : BP005400.D
Acq On : 23 Apr 2021 18:48
Operator : CG/JU
Sample : M2149-16
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-40-9.5-10.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.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
n-Hexadecanoic ...	17.975	10.3	ng	166567	4	17.069	323356	20.0
Octadecanoic acid	19.210	3.5	ng	85940	5	21.175	495851	20.0
unknown19.475	19.475	3.0	ng	73525	5	21.175	495851	20.0
Fumaric acid, 2...	20.886	17.0	ng	421022	5	21.175	495851	20.0
Diethylene glyc...	20.957	3.4	ng	85253	5	21.175	495851	20.0
Oxirane, tetrad...	21.498	3.7	ng	91948	5	21.175	495851	20.0
1-Docosene	21.775	14.2	ng	352499	5	21.175	495851	20.0
Tetradecanal	22.451	5.2	ng	122092	6	23.433	472315	20.0
1-Nonadecene	22.786	5.0	ng	119339	6	23.433	472315	20.0
.gamma.-Tocopherol	23.863	6.7	ng	157771	6	23.433	472315	20.0