

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012624\
Data File : BP019457.D
Acq On : 26 Jan 2024 20:44
Operator : MA/JU
Sample : P1240-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11985

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-BP012624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019457.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	400	408	420	rBV	1217143	1804919	47.12%	7.668%
2	7.081	671	679	688	rBV	1204489	1948462	50.87%	8.278%
3	7.916	812	821	828	rVB	272575	440385	11.50%	1.871%
4	9.081	1011	1019	1027	rBV	736019	1234735	32.23%	5.246%
5	10.716	1288	1297	1304	rBV	337125	593818	15.50%	2.523%
6	13.181	1707	1716	1729	rBV	1634105	2519150	65.77%	10.702%
7	14.510	1937	1942	1943	rBV2	36389	45135	1.18%	0.192%
8	14.545	1943	1948	1955	rVB	503108	781035	20.39%	3.318%
9	16.039	2192	2202	2213	rVB	1299248	1913220	49.95%	8.128%
10	16.716	2312	2317	2322	rBV3	29736	42618	1.11%	0.181%
11	17.304	2410	2417	2422	rBV	679009	984939	25.71%	4.184%
12	17.345	2422	2424	2431	rVV	79271	111965	2.92%	0.476%
13	17.439	2435	2440	2445	rVB	38533	62626	1.63%	0.266%
14	17.492	2445	2449	2456	rBV4	26420	43573	1.14%	0.185%
15	18.086	2545	2550	2557	rBV2	39692	61196	1.60%	0.260%
16	18.216	2567	2572	2581	rBV	408430	578112	15.09%	2.456%
17	19.316	2754	2759	2769	rBV	173175	306842	8.01%	1.304%
18	19.451	2778	2782	2789	rBV2	132975	183812	4.80%	0.781%
19	19.639	2806	2814	2815	rBV2	46374	84406	2.20%	0.359%
20	19.669	2815	2819	2825	rVB	113289	165933	4.33%	0.705%
21	19.874	2849	2854	2864	rVB	3034857	3830515	100.00%	16.274%
22	20.968	3036	3040	3045	rBV	213303	250322	6.53%	1.063%
23	21.133	3063	3068	3075	rBV2	255607	336389	8.78%	1.429%
24	21.339	3098	3103	3107	rBV	522139	606300	15.83%	2.576%
25	21.398	3107	3113	3118	rVV	835501	1244658	32.49%	5.288%
26	21.439	3118	3120	3127	rVB	75660	86052	2.25%	0.366%
27	22.068	3224	3227	3234	rVB3	40815	66442	1.73%	0.282%
28	22.339	3268	3273	3278	rBV	301514	409604	10.69%	1.740%
29	22.721	3332	3338	3346	rVB	657179	1011649	26.41%	4.298%
30	23.086	3395	3400	3405	rBV	55785	127112	3.32%	0.540%
31	23.198	3415	3419	3428	rVB2	74059	132383	3.46%	0.562%
32	23.610	3485	3489	3498	rVB	40711	80872	2.11%	0.344%
33	23.715	3503	3507	3515	rVB	43842	90056	2.35%	0.383%
34	23.827	3518	3526	3545	rVB	566806	1222833	31.92%	5.195%
35	24.662	3662	3668	3676	rBV4	55106	136080	3.55%	0.578%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

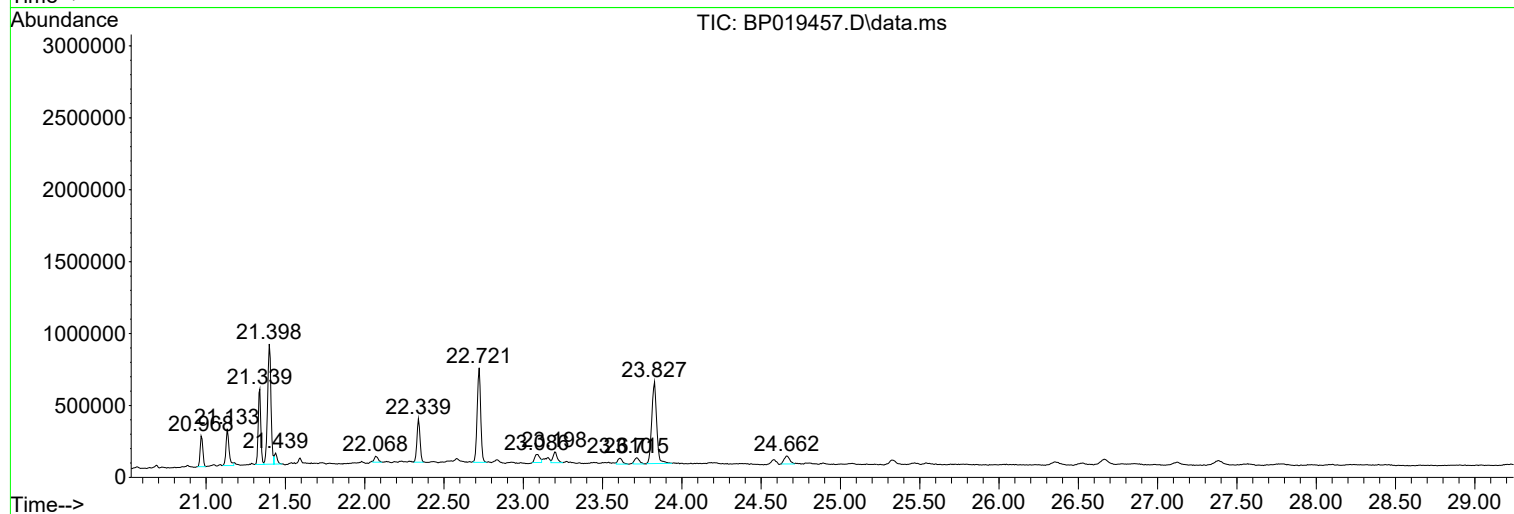
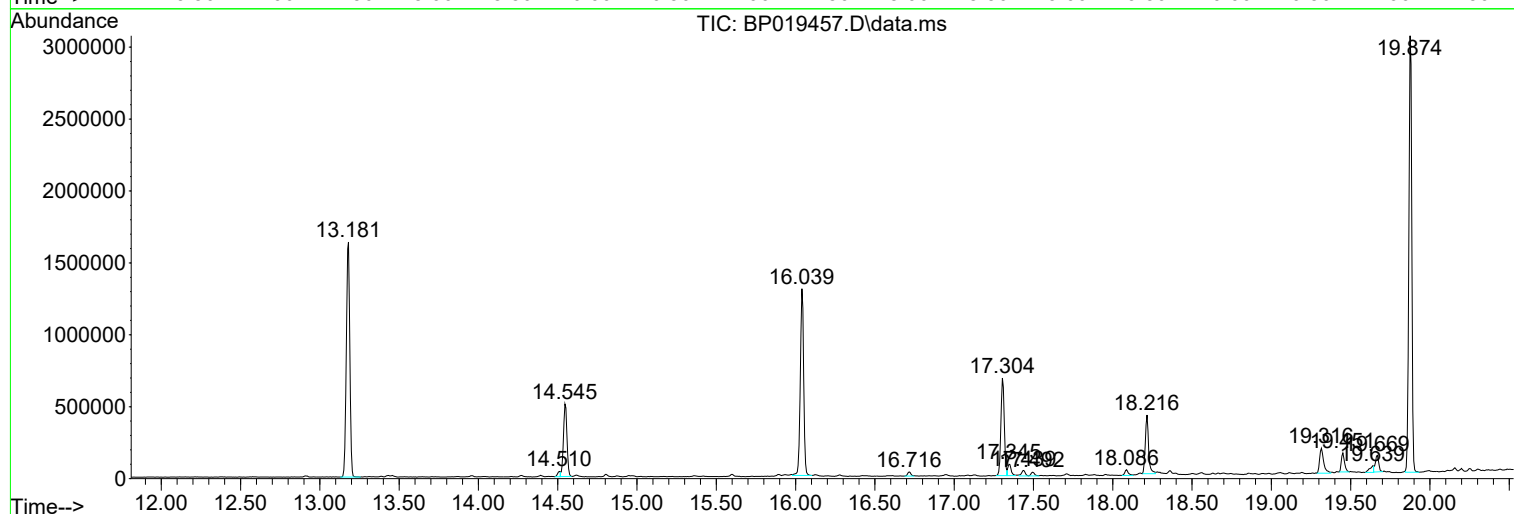
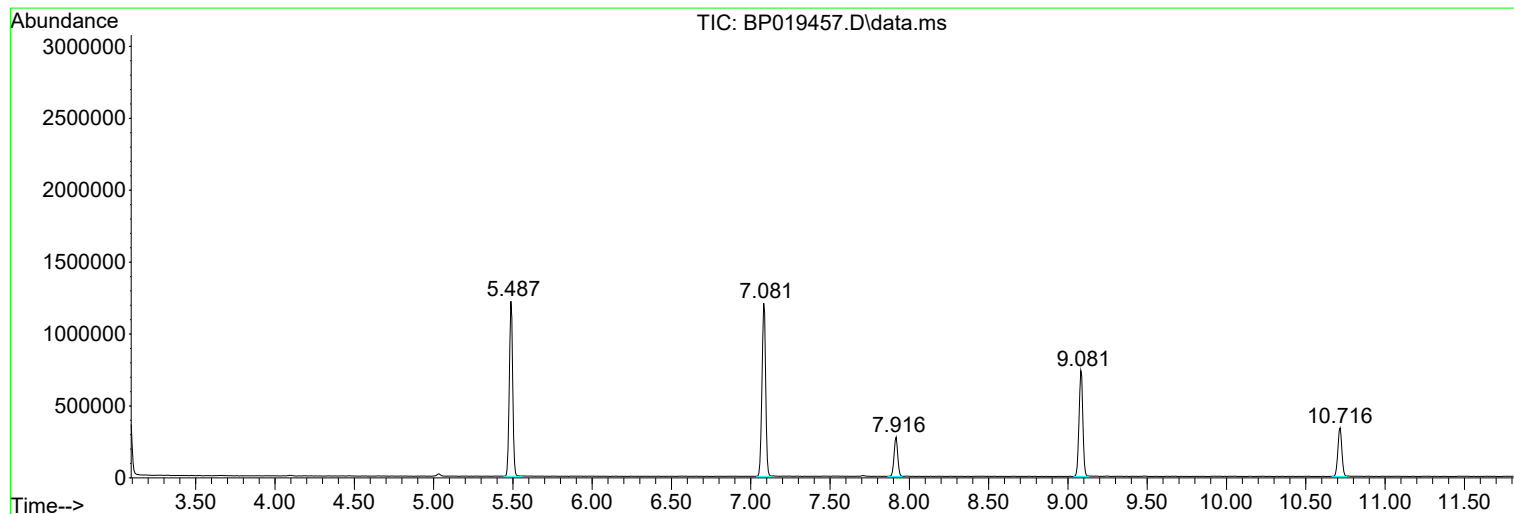
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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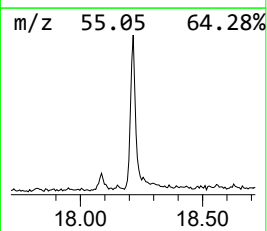
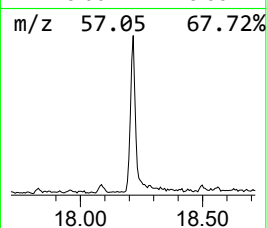
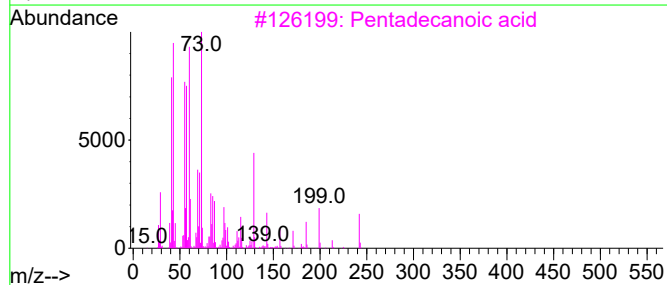
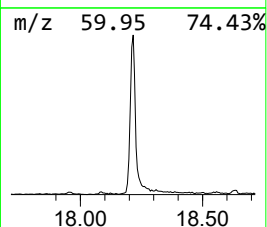
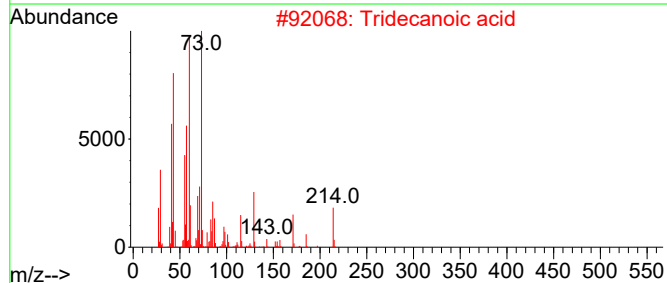
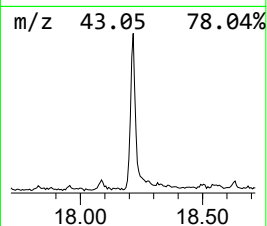
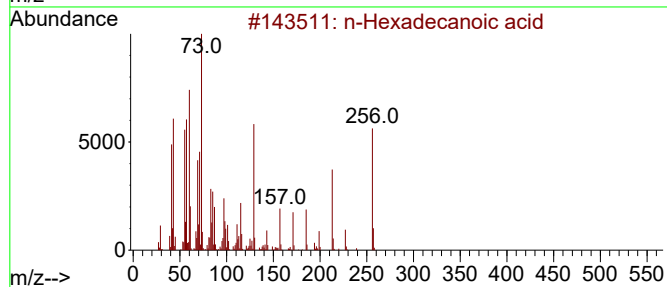
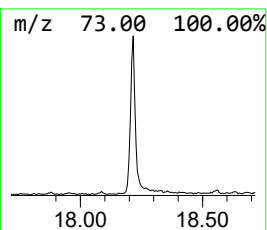
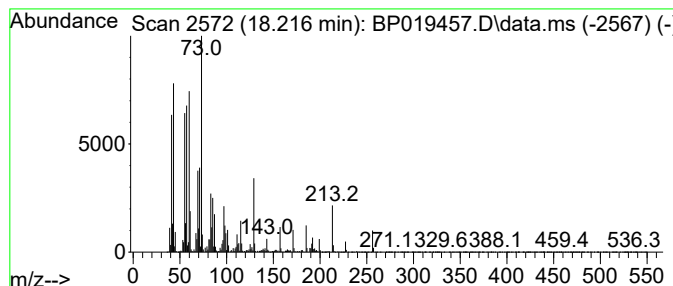
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	11.74 ng	578112	Phenanthrene-d10	17.304

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



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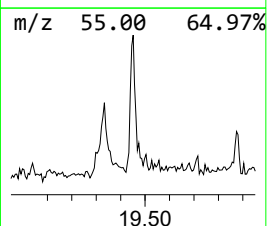
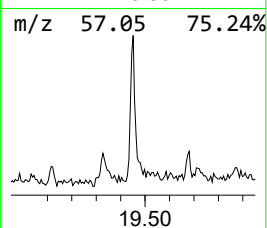
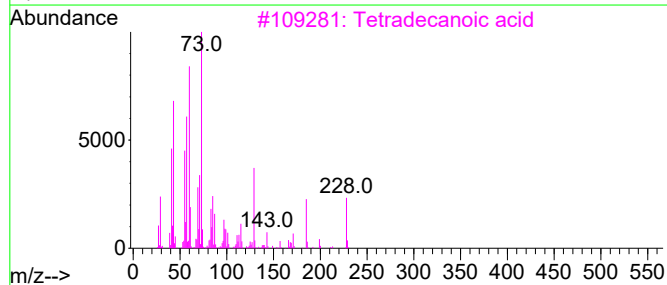
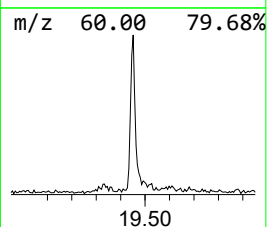
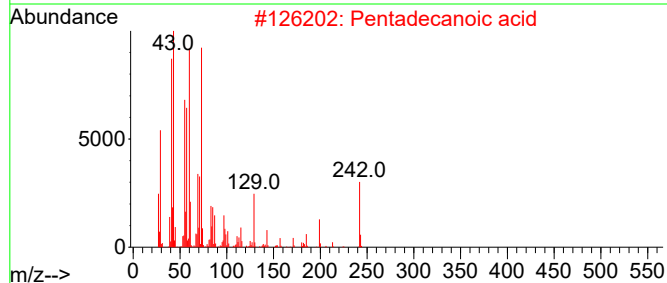
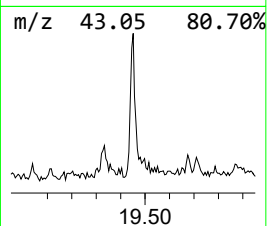
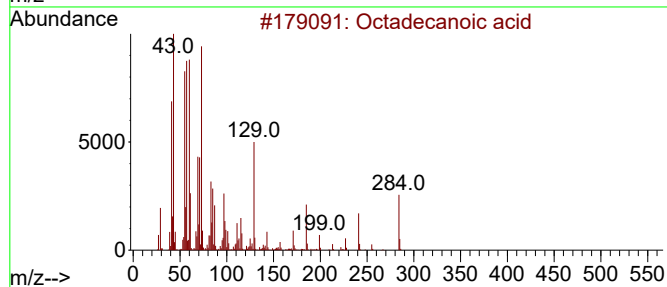
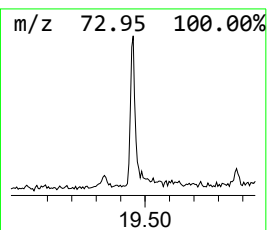
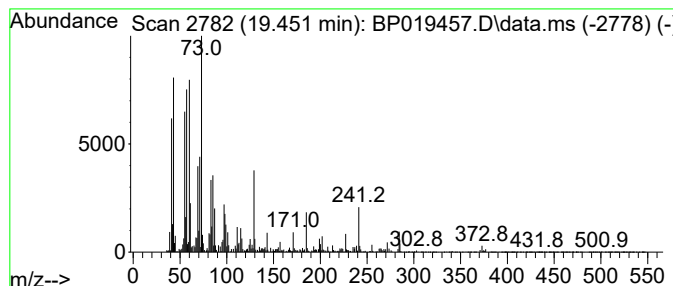
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	2.95 ng	183812	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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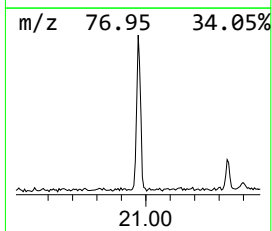
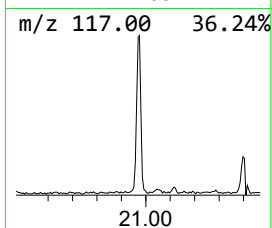
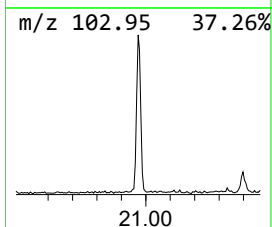
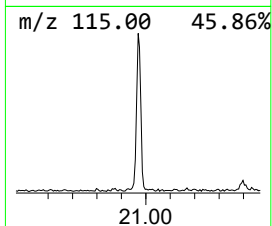
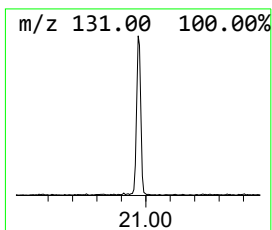
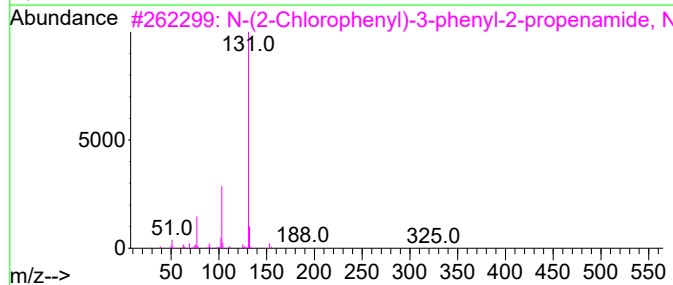
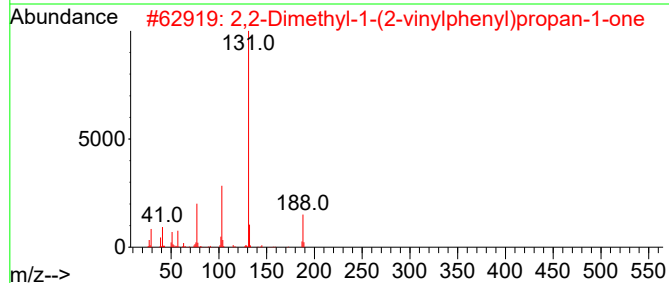
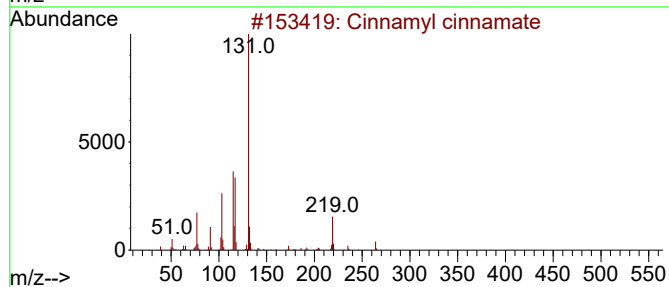
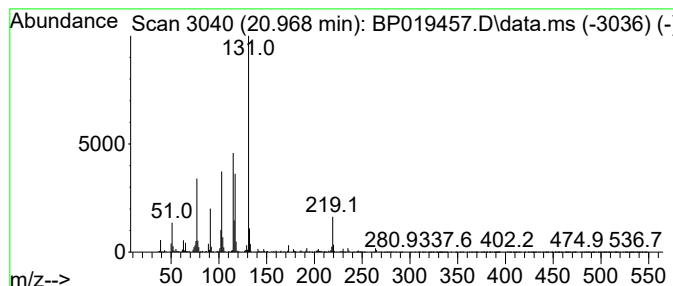
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cinnamyl cinnamate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.968	4.02 ng	250322	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	47
3			N-(2-Chlorophenyl)-3-phenyl-2-pr...	353	C17H11ClF3NO2	1000492-36-9	47
4			2-Propenoic acid, 3-phenyl-, phe...	224	C15H12O2	025695-77-6	47
5			N-[(2Z)-3-Phenylprop-2-enoyl]gly...	233	C13H15NO3	1000498-00-6	47



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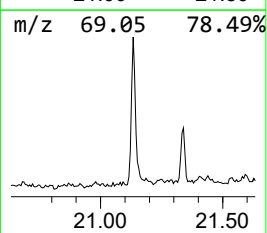
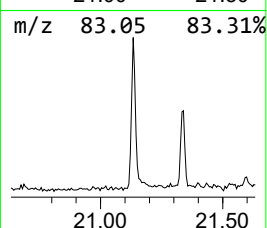
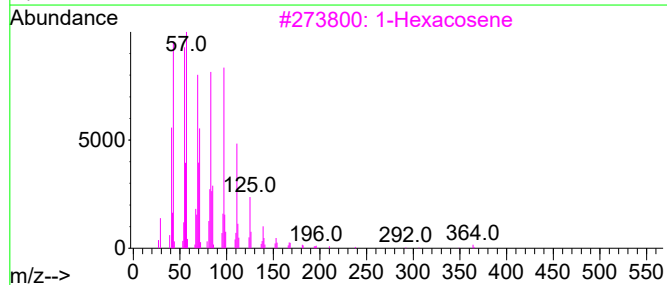
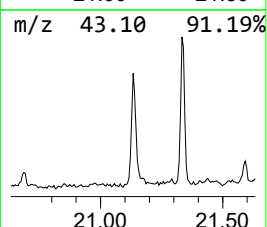
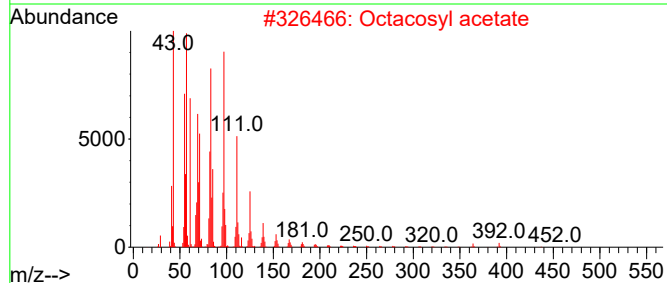
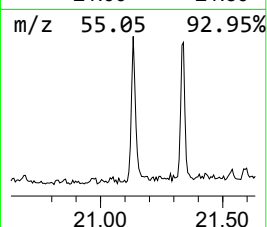
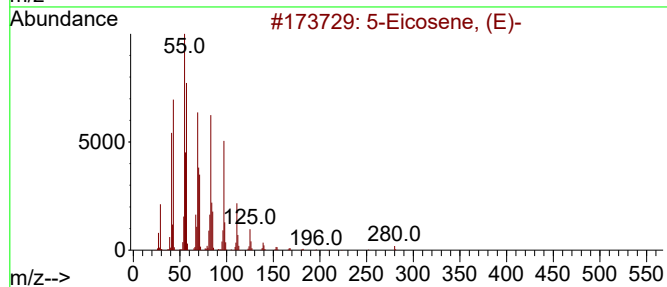
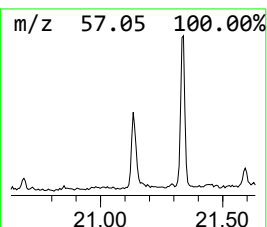
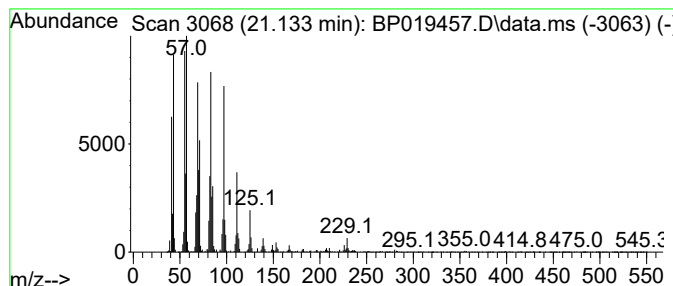
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	5.41 ng	336389	Chrysene-d12	21.398

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2		Octacosyl acetate	452	C30H60O2	018206-97-8	95
3		1-Hexacosene	364	C26H52	018835-33-1	94
4		Nonacos-1-ene	406	C29H58	018835-35-3	94
5		Pentacos-1-ene	350	C25H50	016980-85-1	94



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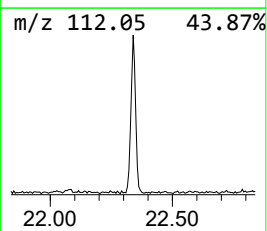
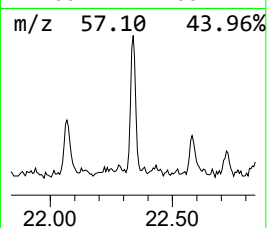
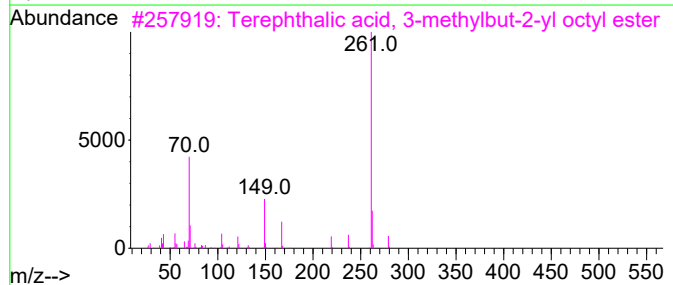
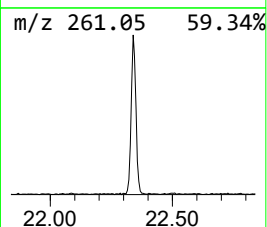
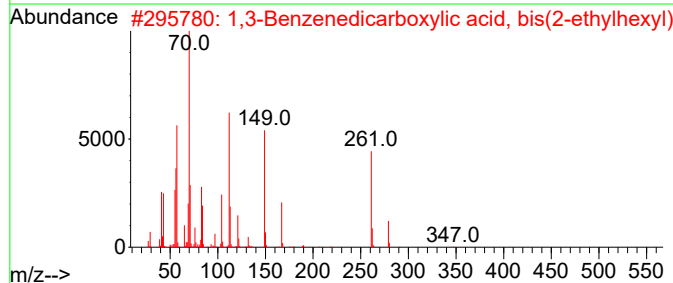
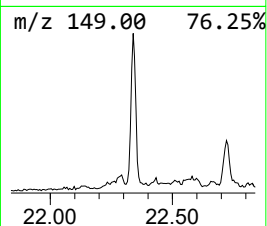
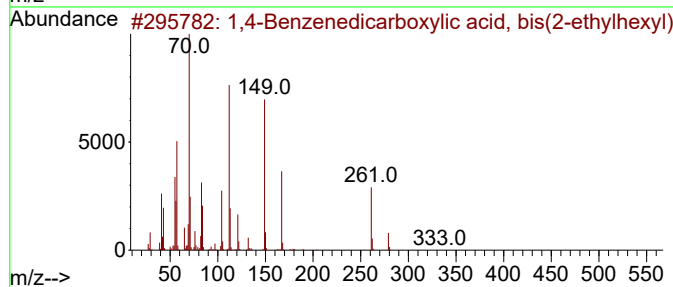
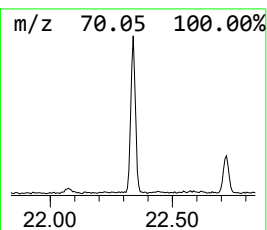
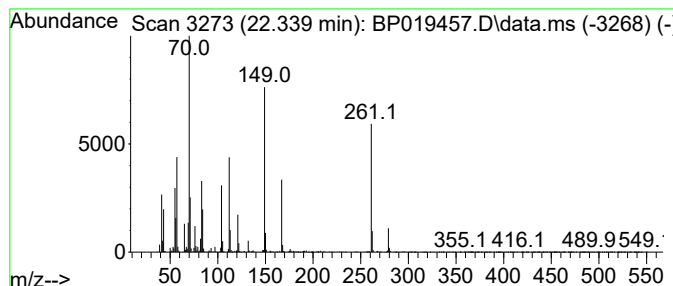
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Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.339	6.58 ng	409604	Chrysene-d12	21.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	72
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	58
3			Terephthalic acid, 3-methylbut-2...	348	C21H3204	1000356-27-6	47
4			Terephthalic acid, 2-ethylhexyl ...	390	C24H3804	1000324-00-5	47
5			Isophthalic acid, di(4-octyl) ester	390	C24H3804	1000344-04-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012624\
Data File : BP019457.D
Acq On : 26 Jan 2024 20:44
Operator : MA/JU
Sample : P1240-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11985

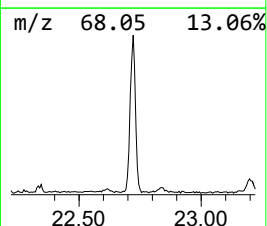
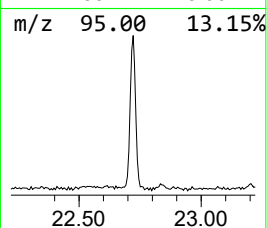
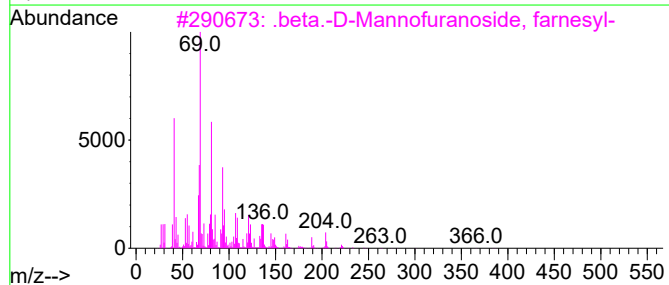
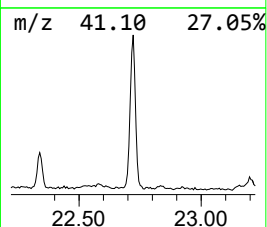
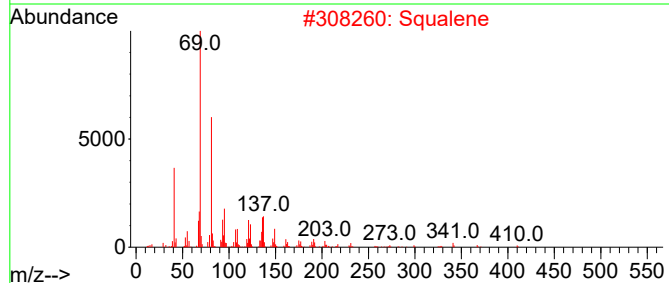
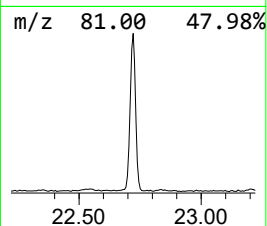
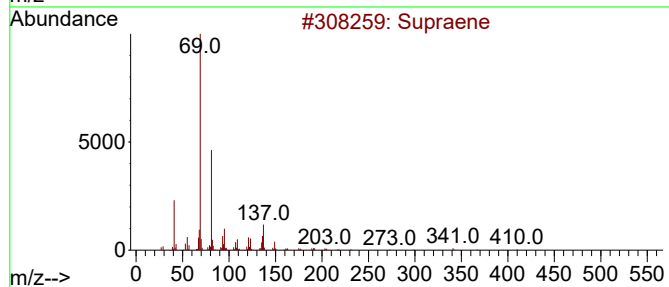
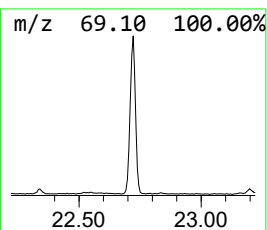
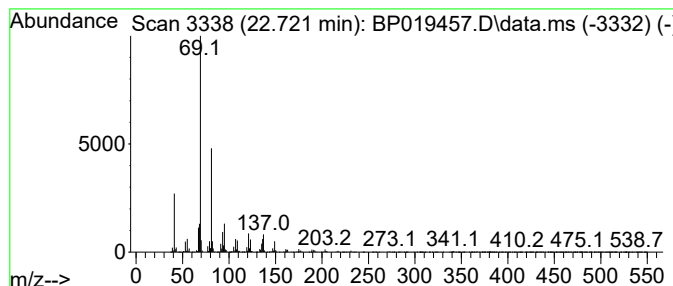
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.721	16.55 ng	1011650	Perylene-d12	23.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	90
3			.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	83
4			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
5			trans-Farnesol	222	C15H26O	000106-28-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012624\
Data File : BP019457.D
Acq On : 26 Jan 2024 20:44
Operator : MA/JU
Sample : P1240-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11985

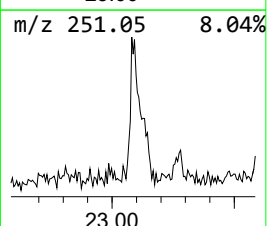
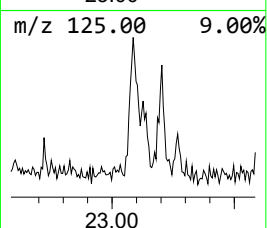
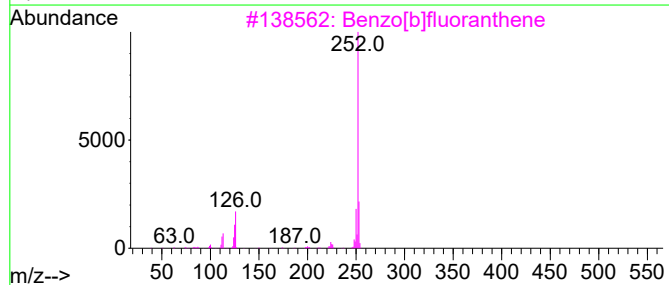
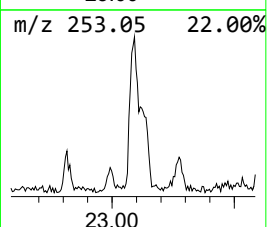
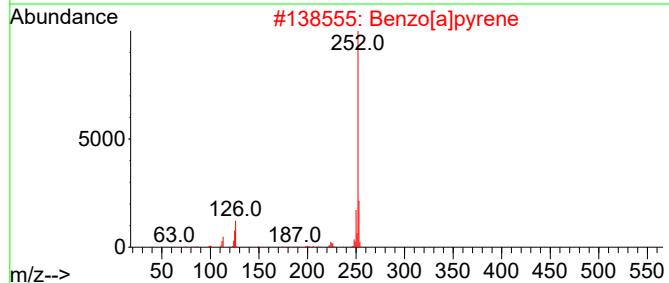
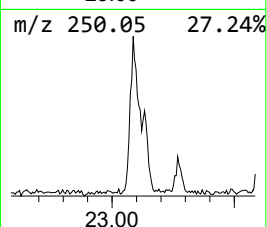
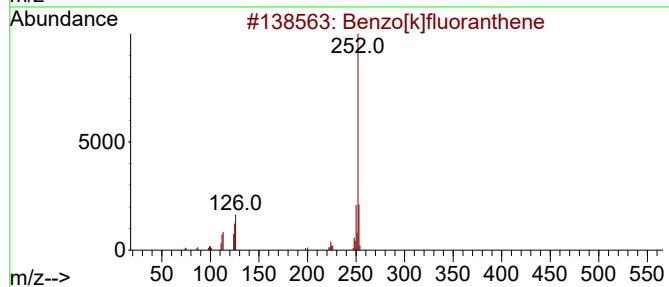
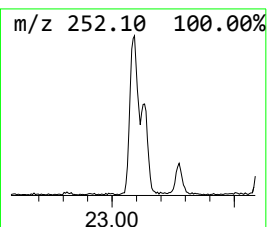
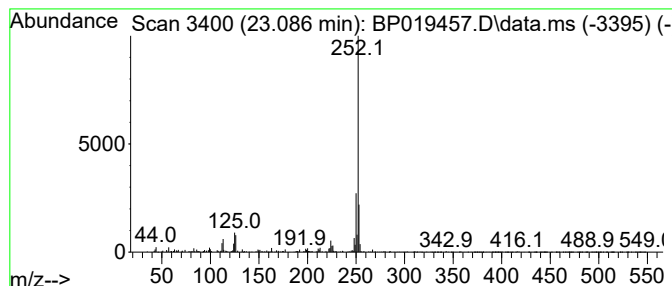
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.086	2.08 ng	127112	Perylene-d12	23.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
2			Benzo[a]pyrene	252	C20H12	000050-32-8	93
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
4			Benzo[e]pyrene	252	C20H12	000192-97-2	90
5			Perylene	252	C20H12	000198-55-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012624\
Data File : BP019457.D
Acq On : 26 Jan 2024 20:44
Operator : MA/JU
Sample : P1240-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11985

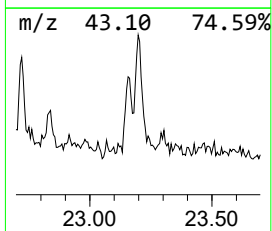
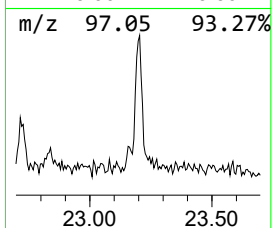
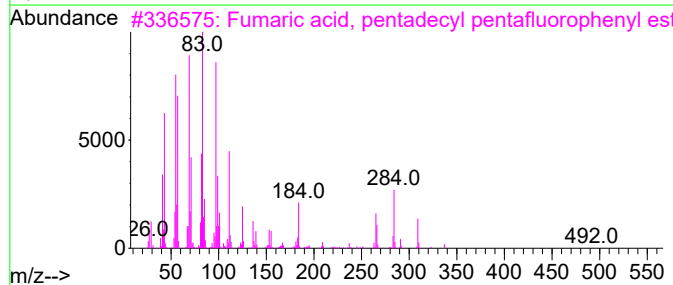
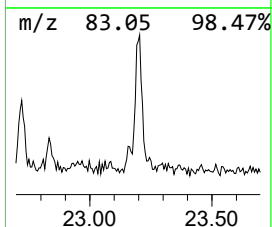
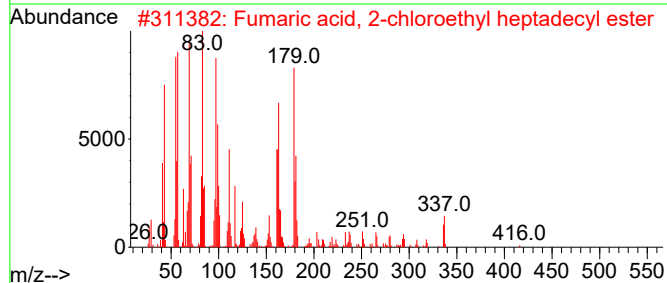
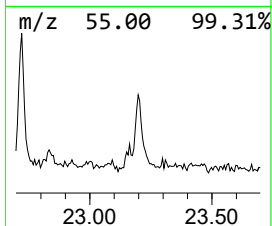
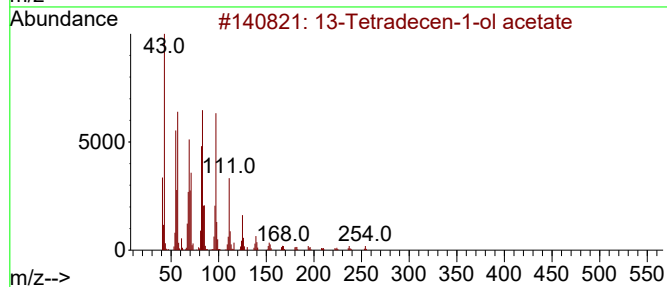
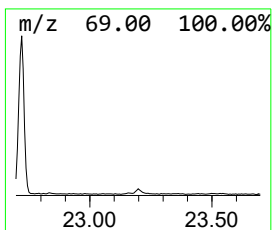
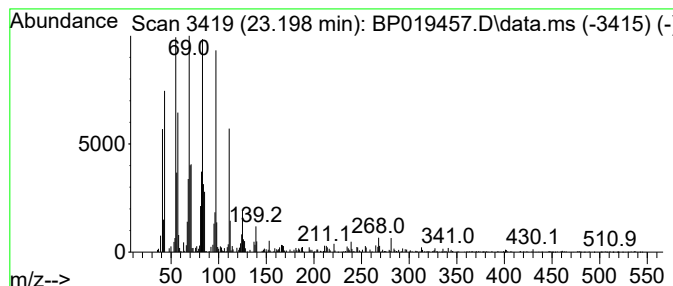
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Tetradecen-1-ol acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.198	2.17 ng	132383	Perylene-d12	23.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
2			Fumaric acid, 2-chloroethyl hept...	416	C23H41ClO4	1000330-62-3	90
3			Fumaric acid, pentadecyl pentafl...	492	C25H33F5O4	1000348-10-7	80
4			1-Heneicosanol	312	C21H44O	015594-90-8	76
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012624\
Data File : BP019457.D
Acq On : 26 Jan 2024 20:44
Operator : MA/JU
Sample : P1240-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11985

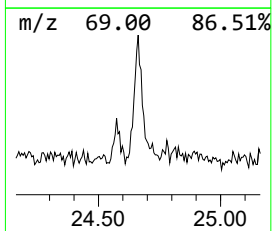
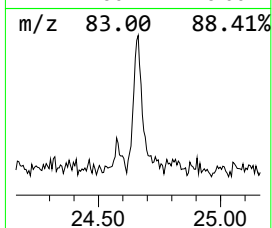
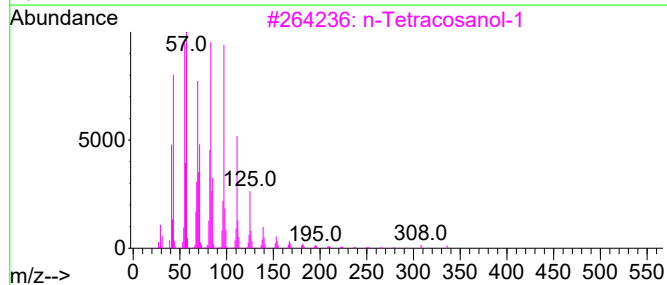
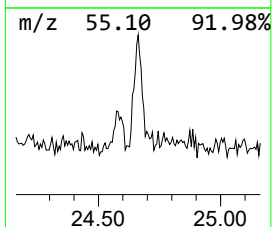
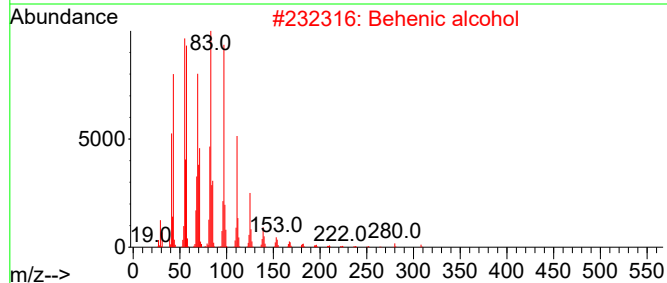
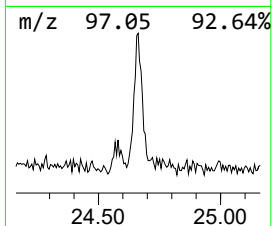
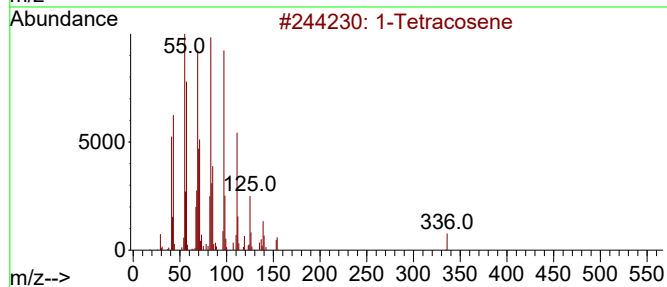
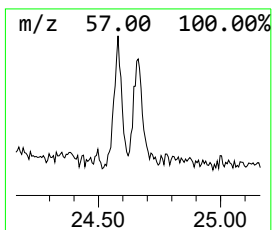
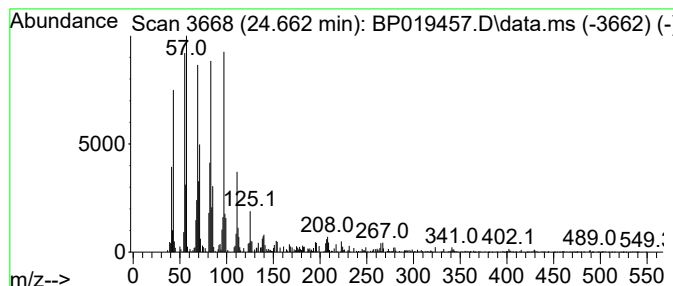
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Tetracosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.662	2.23 ng	136080	Perylene-d12	23.827

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetracosene	336	C24H48	010192-32-2	98
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4		Octacosanol	410	C28H58O	000557-61-9	91
5		1-Heptacosanol	396	C27H56O	002004-39-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012624\
Data File : BP019457.D
Acq On : 26 Jan 2024 20:44
Operator : MA/JU
Sample : P1240-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012624.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
n-Hexadecanoic ...	18.216	11.7	ng	578112	4	17.304	984939	20.0
Octadecanoic acid	19.451	3.0	ng	183812	5	21.398	1244660	20.0
Cinnamyl cinnamate	20.968	4.0	ng	250322	5	21.398	1244660	20.0
5-Eicosene, (E)-	21.133	5.4	ng	336389	5	21.398	1244660	20.0
1,4-Benzenedica...	22.339	6.6	ng	409604	5	21.398	1244660	20.0
Supraene	22.721	16.6	ng	1011650	6	23.827	1222830	20.0
Benzo[e]pyrene	23.086	2.1	ng	127112	6	23.827	1222830	20.0
13-Tetradecen-1...	23.198	2.2	ng	132383	6	23.827	1222830	20.0
1-Tetracosene	24.662	2.2	ng	136080	6	23.827	1222830	20.0