

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
 Data File : BF136984.D
 Acq On : 05 Jan 2024 19:32
 Operator : CG\JU
 Sample : 05967-08
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COLT1

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_F\Methods\8270-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	10	14	22	rVB	23552	33036	2.26%	0.415%
2	5.010	493	497	509	rBV	230852	229225	15.68%	2.878%
3	5.428	565	568	584	rBV	467329	454924	31.13%	5.711%
4	6.434	736	739	755	rBV	310068	306525	20.97%	3.848%
5	6.781	795	798	802	rBV	356093	298287	20.41%	3.745%
6	7.345	890	894	897	rBV	865368	741967	50.77%	9.315%
7	8.057	1012	1015	1019	rBV	377044	341247	23.35%	4.284%
8	9.139	1194	1199	1202	rBV	1601954	1350249	92.39%	16.951%
9	9.816	1311	1314	1322	rVB	423595	338306	23.15%	4.247%
10	10.610	1446	1449	1458	rBV	512685	498950	34.14%	6.264%
11	10.981	1509	1512	1519	rBV	99085	96518	6.60%	1.212%
12	11.310	1564	1568	1571	rBV	416582	352003	24.09%	4.419%
13	11.845	1655	1659	1674	rBV	64867	83117	5.69%	1.043%
14	12.010	1684	1687	1691	rVB	24612	25712	1.76%	0.323%
15	12.233	1719	1725	1727	rBV	39399	41942	2.87%	0.527%
16	12.257	1727	1729	1737	rVB	53865	43952	3.01%	0.552%
17	12.522	1767	1774	1776	rBV	73575	104206	7.13%	1.308%
18	12.545	1776	1778	1790	rVB4	52967	100426	6.87%	1.261%
19	12.663	1795	1798	1807	rVB	297767	300322	20.55%	3.770%
20	12.910	1835	1840	1843	rBV	1703239	1461438	100.00%	18.347%
21	13.863	1998	2002	2003	rBV4	24946	29425	2.01%	0.369%
22	13.969	2017	2020	2024	rBV	379732	359377	24.59%	4.512%
23	14.063	2034	2036	2039	rVB2	28818	28961	1.98%	0.364%
24	14.821	2161	2165	2168	rBV	50137	56909	3.89%	0.714%
25	15.457	2269	2273	2281	rBV	221933	288453	19.74%	3.621%

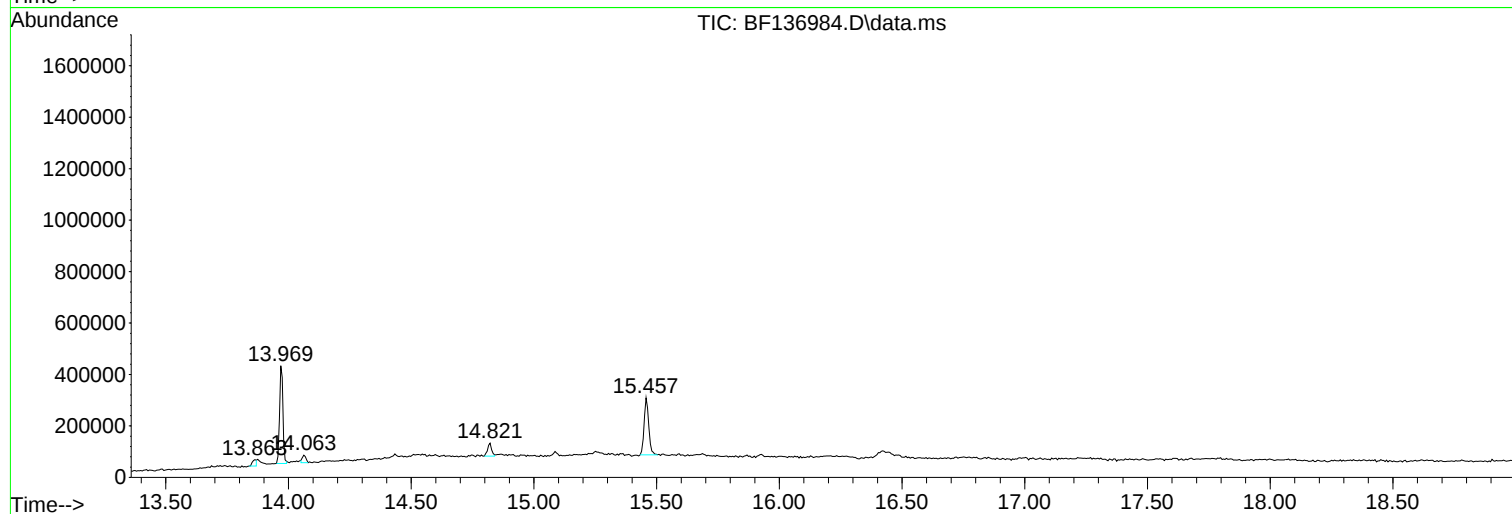
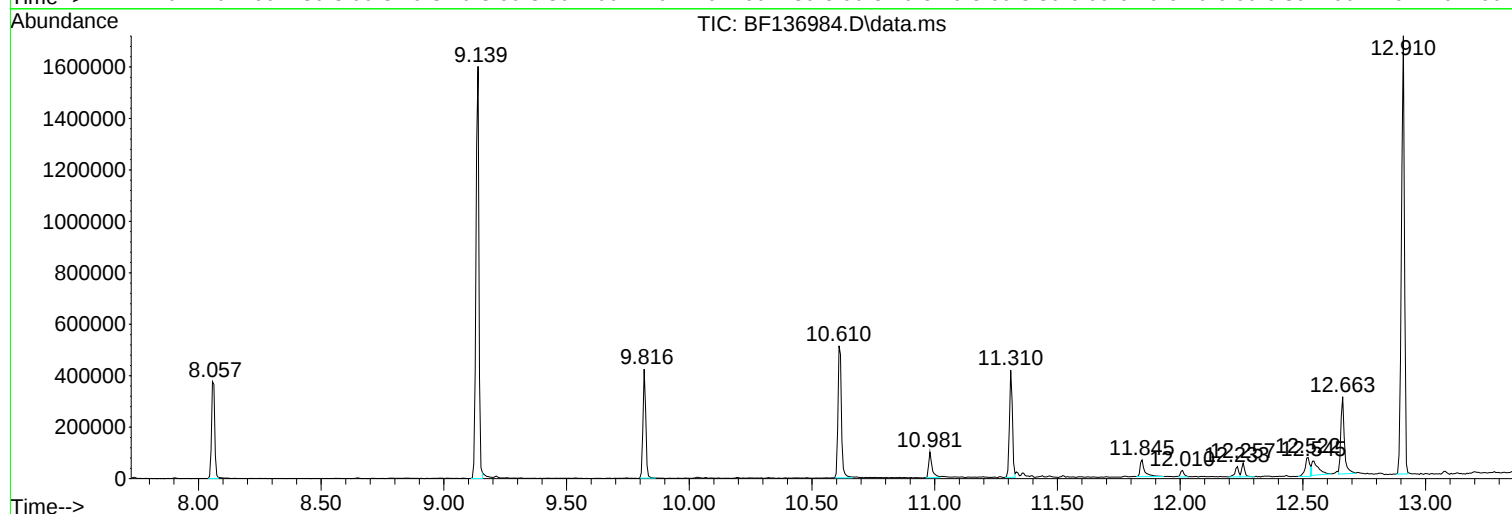
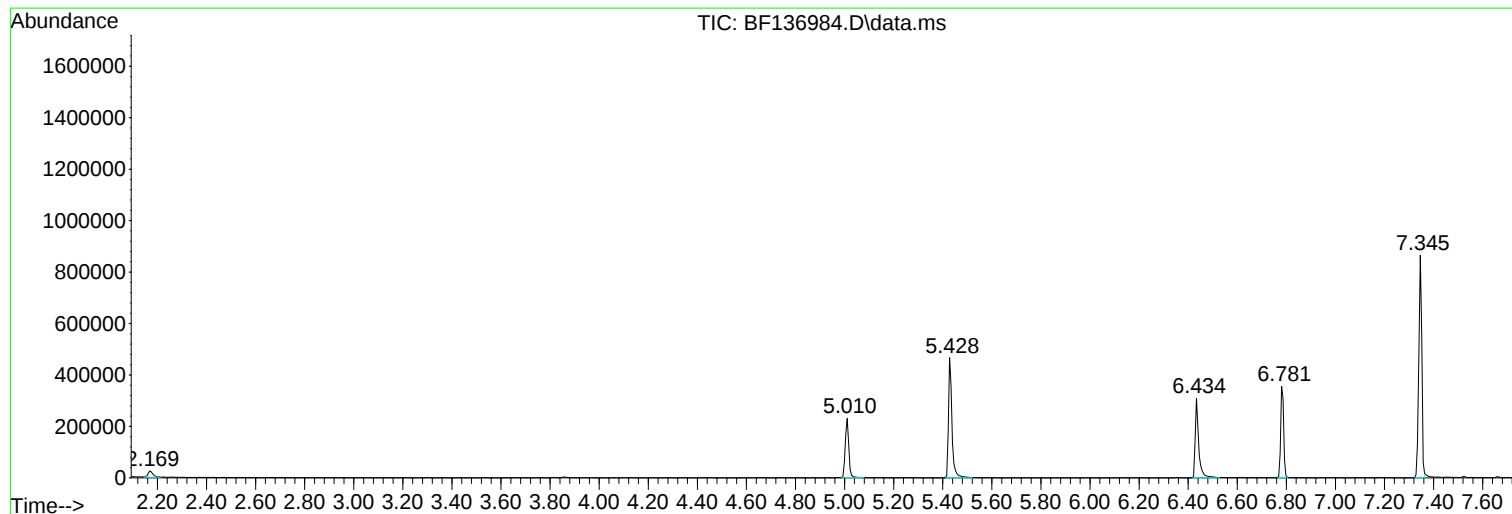
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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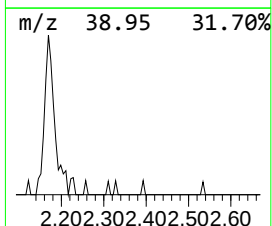
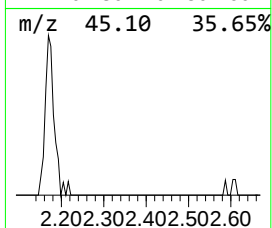
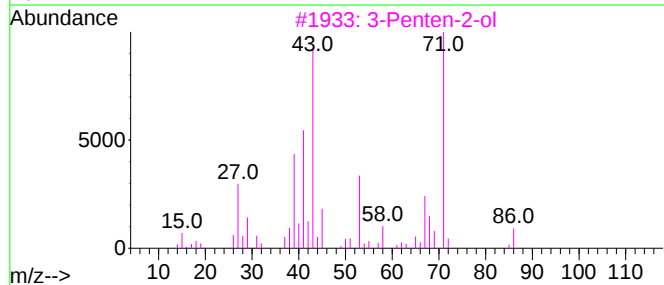
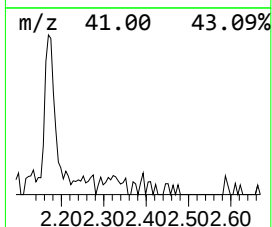
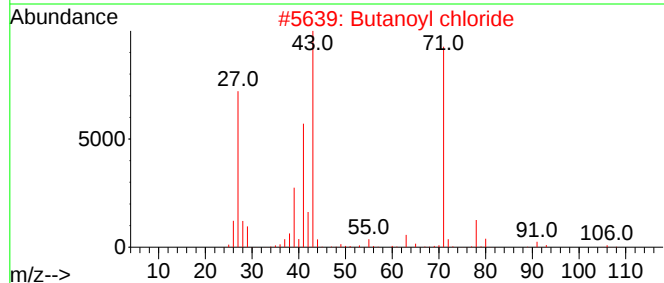
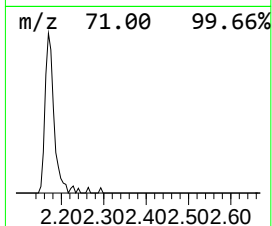
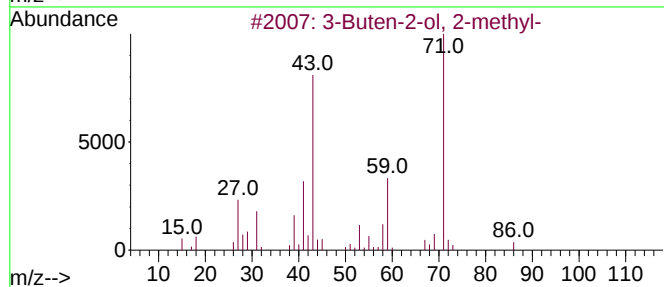
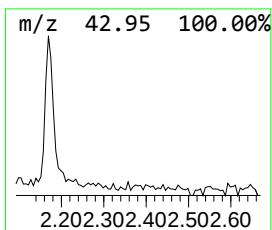
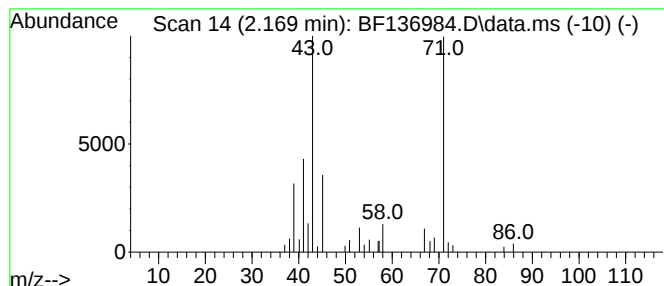
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	2.22 ng	33036	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
2			Butanoyl chloride	106	C4H7ClO	000141-75-3	47
3			3-Penten-2-ol	86	C5H10O	001569-50-2	45
4			Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	42
5			2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	42



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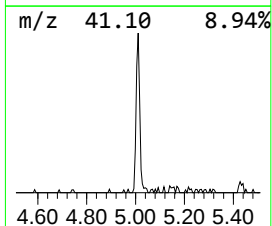
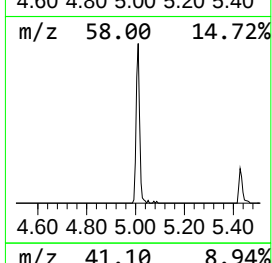
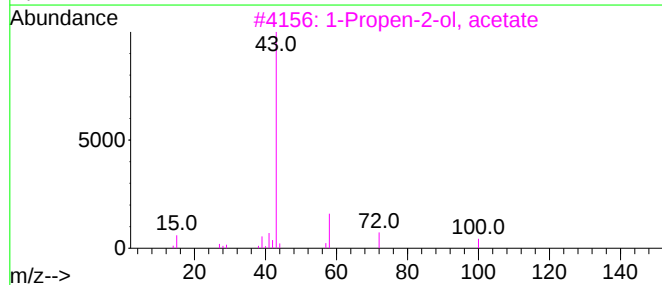
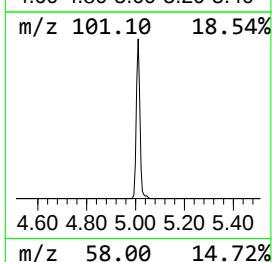
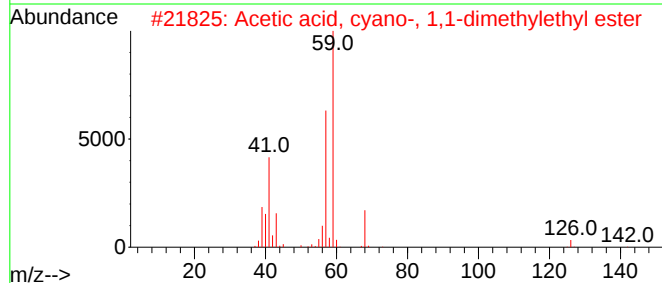
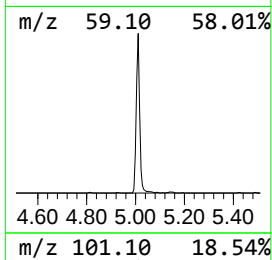
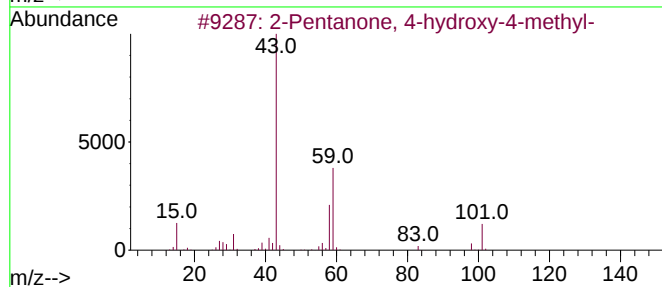
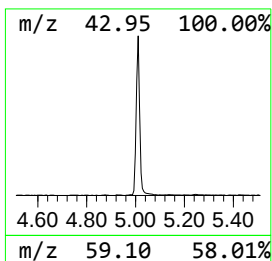
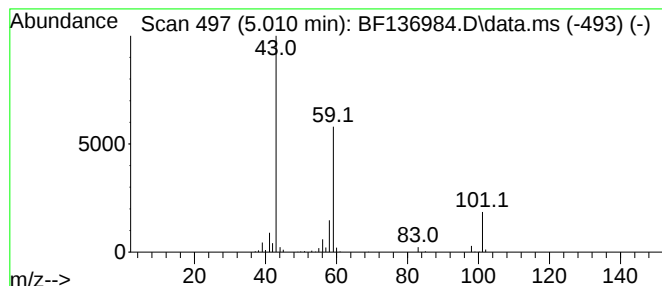
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	15.37 ng	229225	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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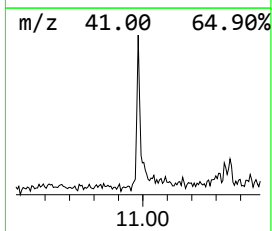
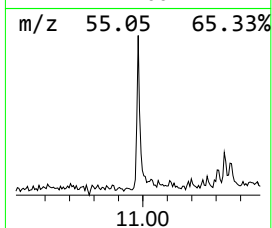
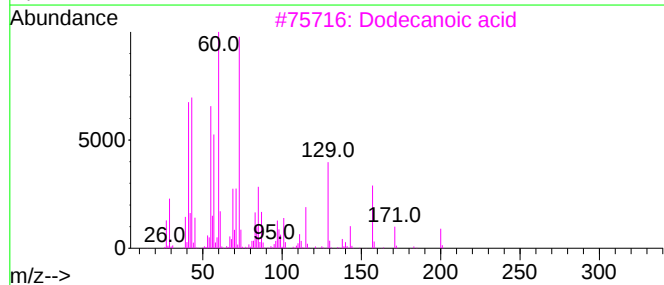
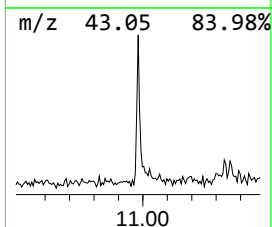
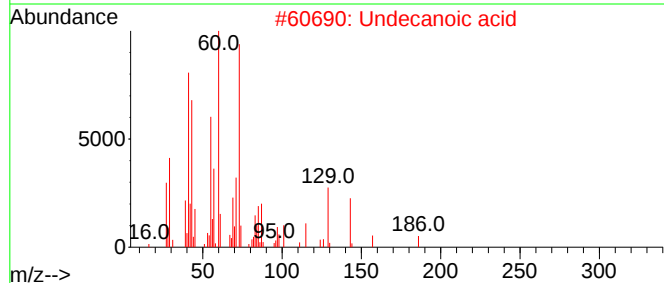
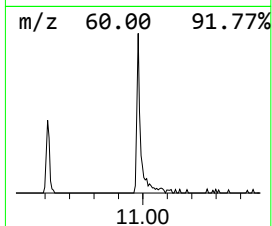
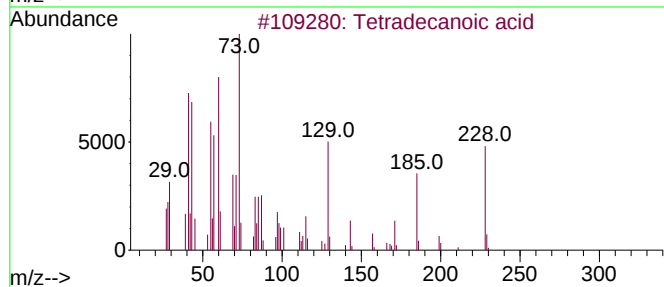
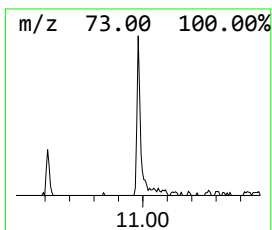
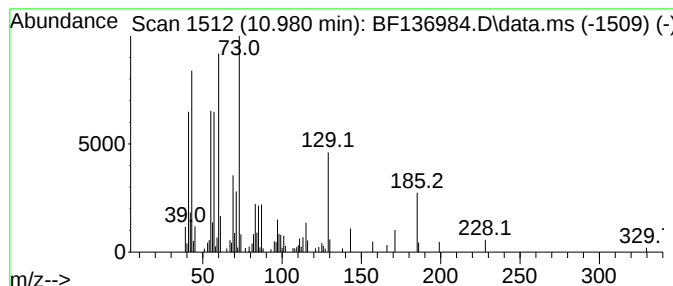
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.980	5.48 ng	96518	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
2			Undecanoic acid	186	C11H22O2	000112-37-8	86
3			Dodecanoic acid	200	C12H24O2	000143-07-7	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



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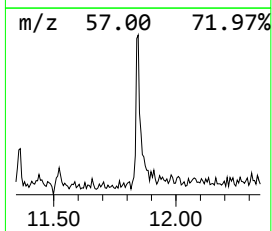
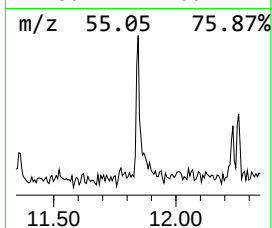
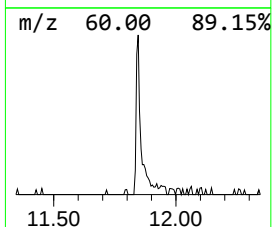
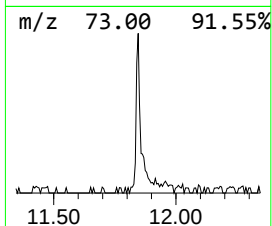
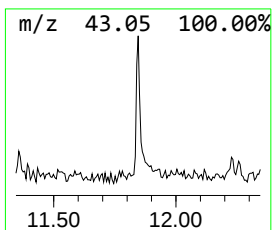
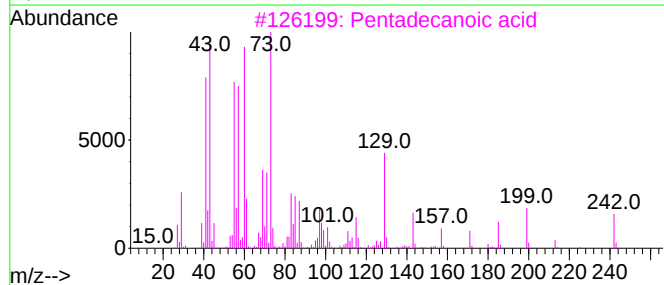
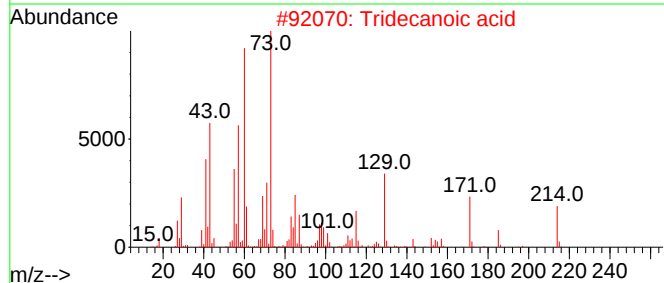
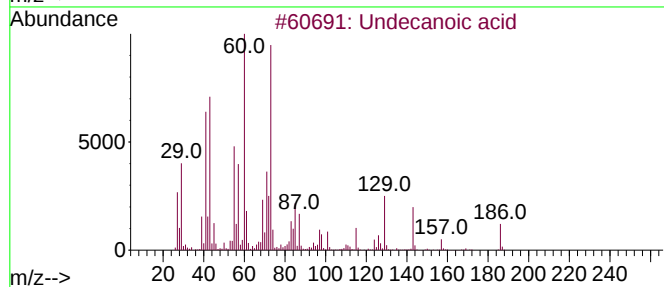
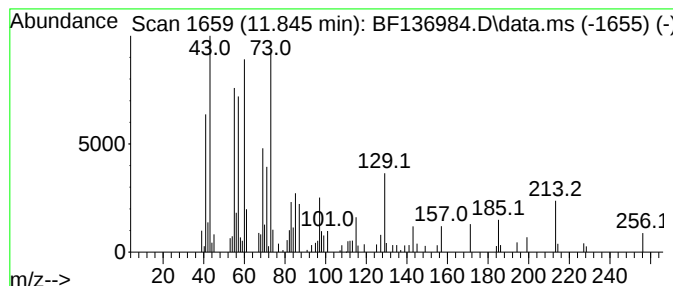
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.845	4.72 ng	83117	Phenanthrene-d10	11.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	83
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55



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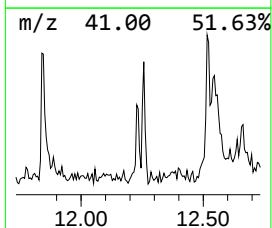
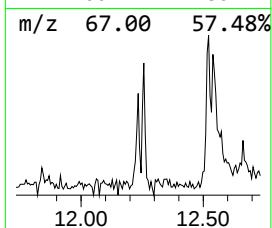
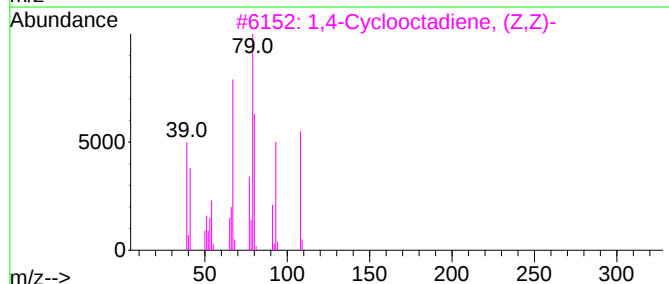
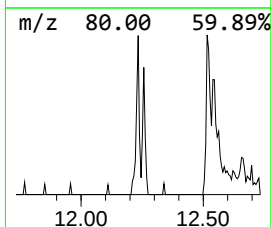
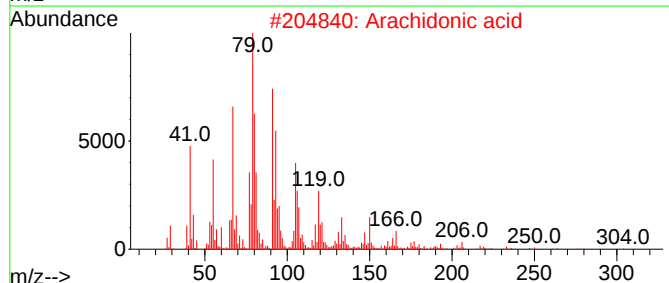
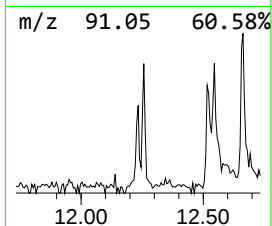
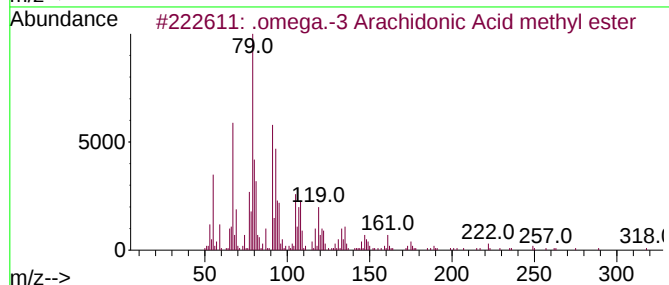
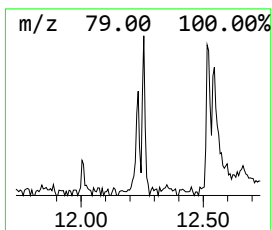
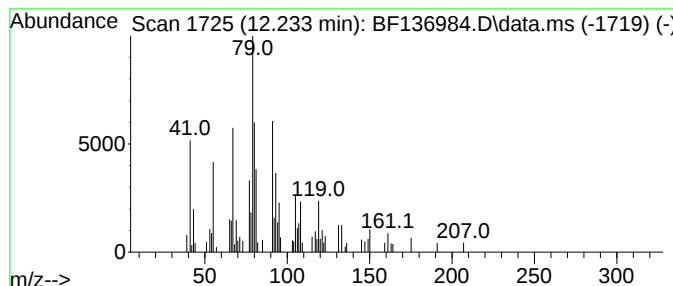
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 5 .omega.-3 Arachidonic Acid ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.233	2.38 ng	41942	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.omega.-3 Arachidonic Acid methy...	318	C21H34O2	132712-70-0	86
2			Arachidonic acid	304	C20H32O2	000506-32-1	83
3			1,4-Cyclooctadiene, (Z,Z)-	108	C8H12	016327-22-3	70
4			Methyl 4,7,10,13-hexadecatetraen...	262	C17H26O2	1000336-36-7	62
5			Cyclopropane, (R,R)-1-((Z)-hex-1...	150	C11H18	077210-40-3	58



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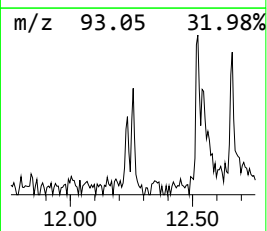
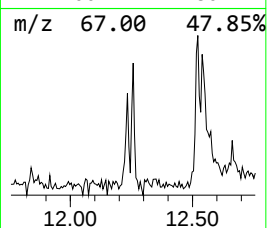
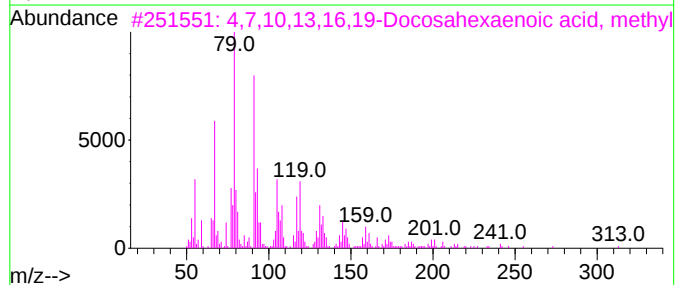
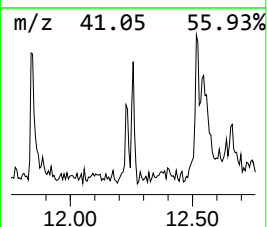
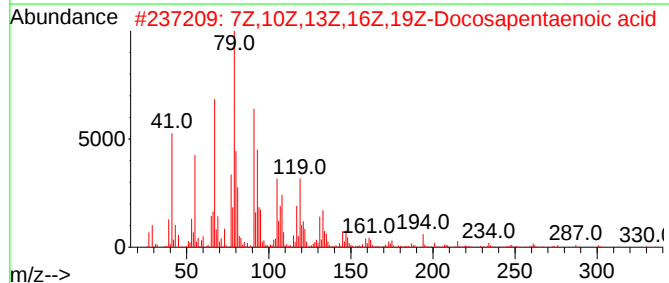
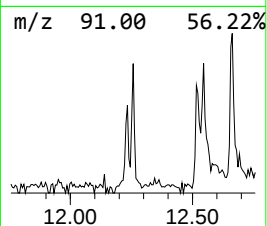
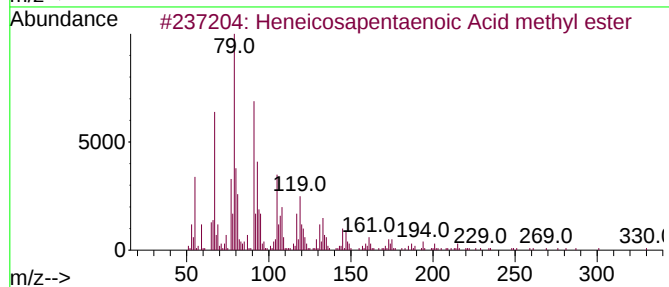
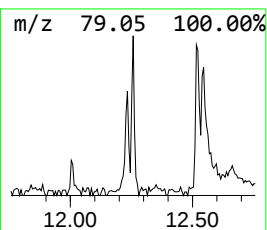
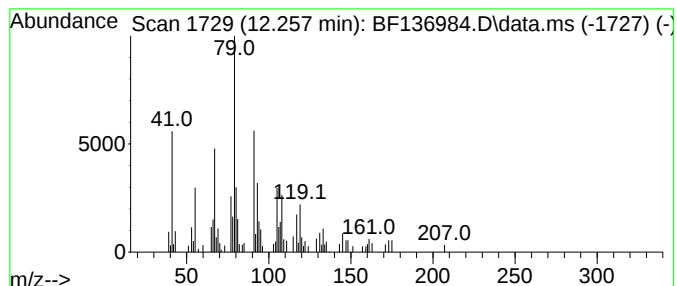
Instrument :
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ClientSampleId :
COLT1

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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 Heneicosapentaenoic Acid me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.257	2.50 ng	43952	Phenanthrene-d10		11.310	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heneicosapentaenoic Acid methyl ...		330	C22H34O2	065919-53-1	78
2	7Z,10Z,13Z,16Z,19Z-Docosapentaen...		330	C22H34O2	024880-45-3	76
3	4,7,10,13,16,19-Docosahexaenoic ...		342	C23H34O2	002566-90-7	62
4	cis-5,8,11,14,17-Eicosapentaenoi...		302	C20H30O2	010417-94-4	50
5	Doconexent		328	C22H32O2	006217-54-5	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136984.D
Acq On : 05 Jan 2024 19:32
Operator : CG\JU
Sample : 05967-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COLT1

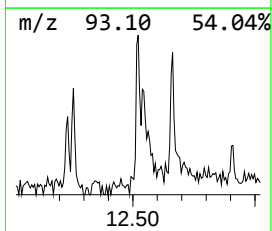
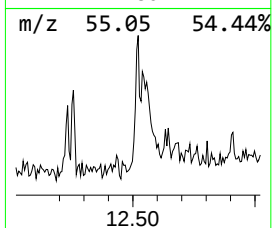
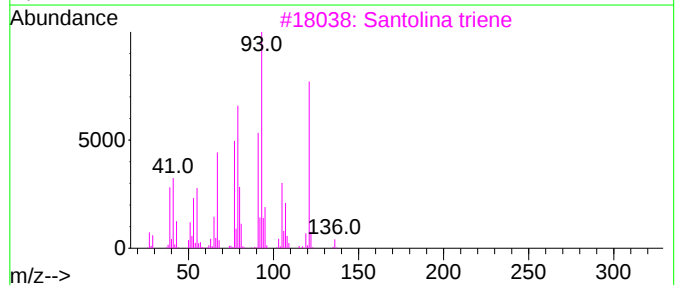
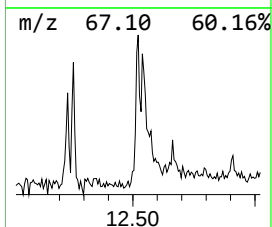
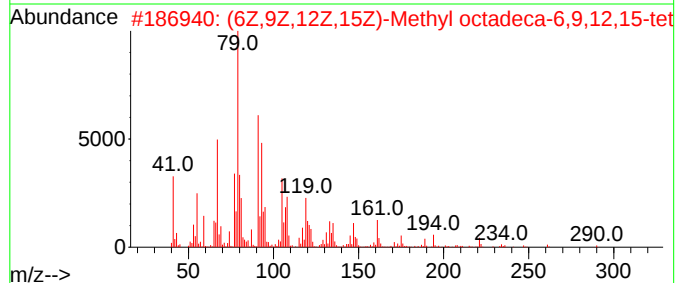
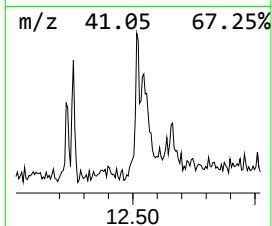
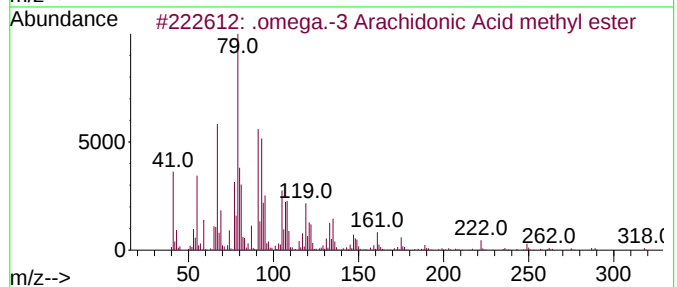
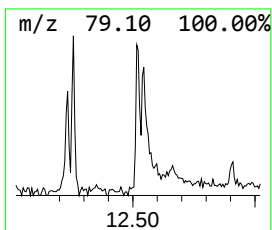
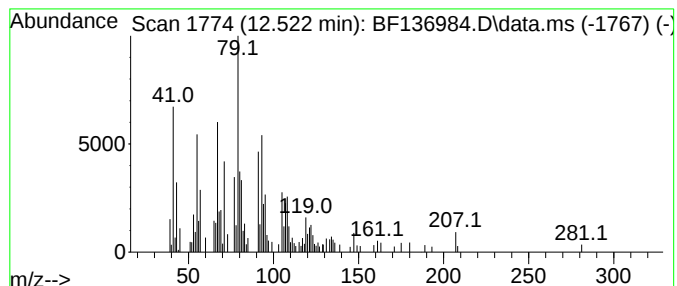
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Santolina triene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	5.92 ng	104206	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	omega.-3	Arachidonic Acid methy...	318	C21H34O2	132712-70-0	81
2	(6Z,9Z,12Z,15Z)-	Methyl octadeca-	...	290	C19H30O2	073097-00-4	64
3	Santolina	triene		136	C10H16	002153-66-4	58
4	1,4,8-	Dodecatriene, (E,E,E)-		162	C12H18	024252-85-5	52
5	Cyclooctene, 3-	ethenyl-		136	C10H16	002213-60-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136984.D
Acq On : 05 Jan 2024 19:32
Operator : CG\JU
Sample : 05967-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COLT1

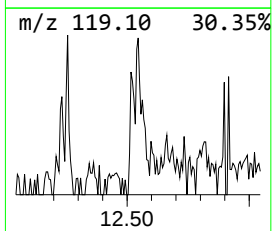
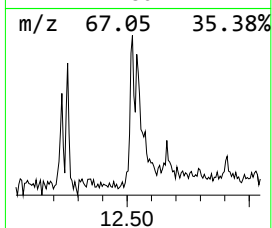
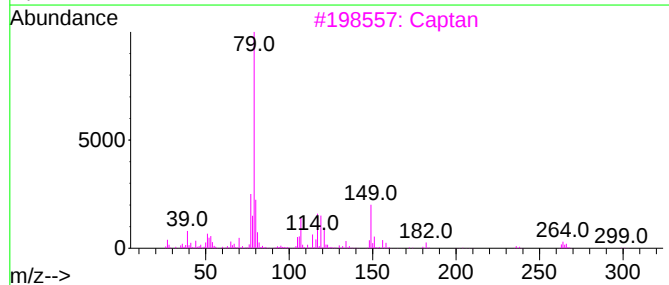
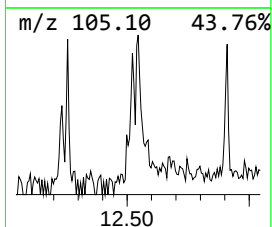
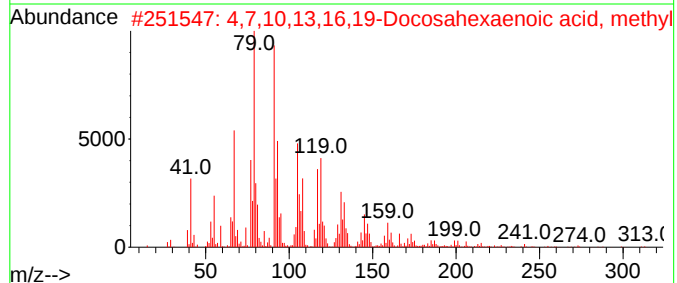
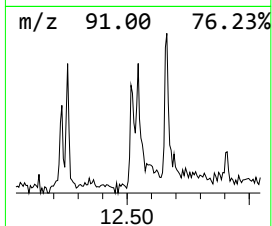
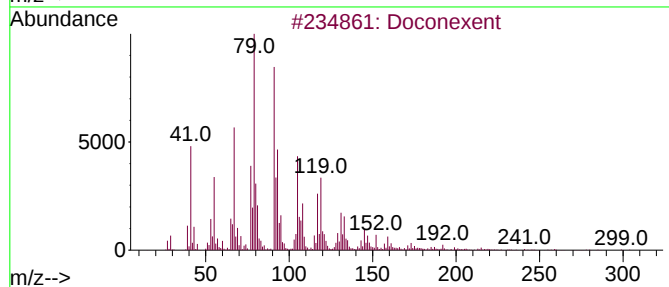
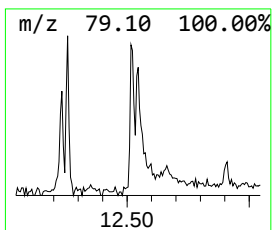
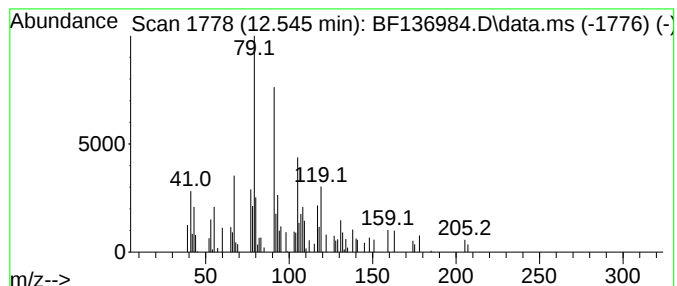
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Doconexent Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	5.71 ng	100426	Phenanthrene-d10	11.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Doconexent	328	C22H32O2	006217-54-5	64
2		4,7,10,13,16,19-Docosahexaenoic ...	342	C23H34O2	002566-90-7	58
3		Captan	299	C9H8Cl3NO2S	000133-06-2	47
4		2-Dodecen-4-yne, (E)-	164	C12H20	074744-38-0	35
5		7Z,10Z,13Z,16Z,19Z-Docosapentaen...	330	C22H34O2	024880-45-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136984.D
Acq On : 05 Jan 2024 19:32
Operator : CG\JU
Sample : 05967-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COLT1

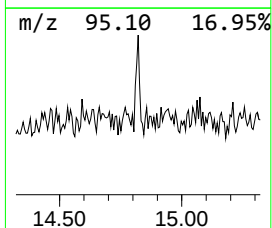
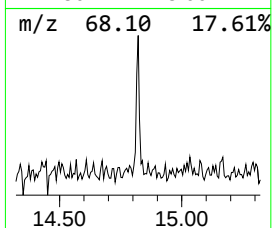
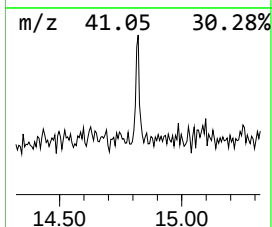
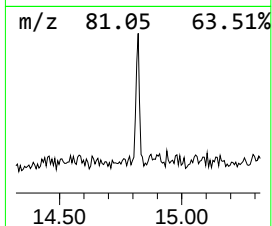
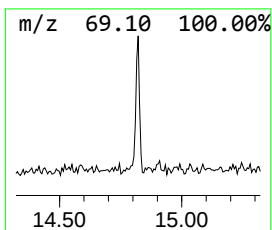
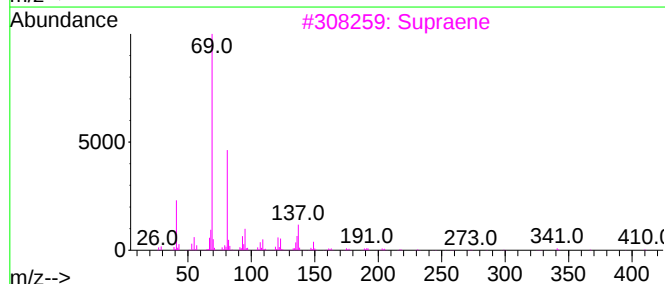
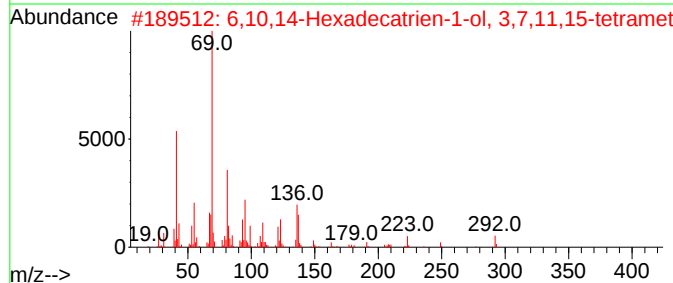
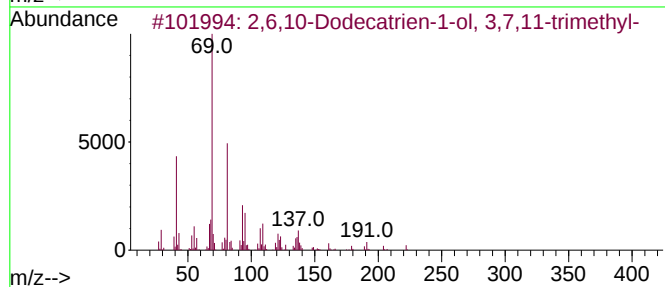
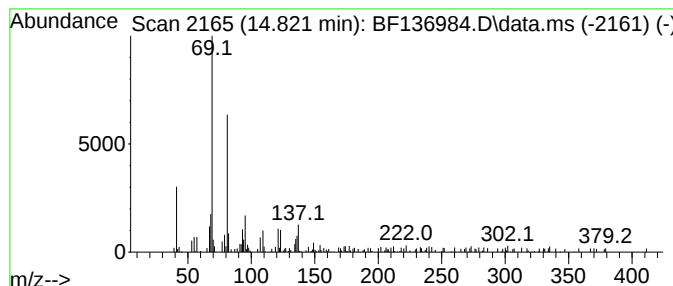
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	3.95 ng	56909	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	86		
2	6,10,14-Hexadecatrien-1-ol, 3,7,...	292	C20H36O	036237-66-8	86		
3	Supraene	410	C30H50	007683-64-9	86		
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83		
5	trans-Farnesol	222	C15H26O	000106-28-5	80		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136984.D
Acq On : 05 Jan 2024 19:32
Operator : CG\JU
Sample : 05967-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COLT1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
3-Buten-2-ol, 2...	2.169	2.2	ng	33036	1	6.781	298287	20.0
2-Pentanone, 4-...	5.010	15.4	ng	229225	1	6.781	298287	20.0
Tetradecanoic acid	10.980	5.5	ng	96518	4	11.310	352003	20.0
Undecanoic acid	11.845	4.7	ng	83117	4	11.310	352003	20.0
.omega.-3 Arach...	12.233	2.4	ng	41942	4	11.310	352003	20.0
Heneicosapentae...	12.257	2.5	ng	43952	4	11.310	352003	20.0
Santolina triene	12.522	5.9	ng	104206	4	11.310	352003	20.0
Doconexent	12.545	5.7	ng	100426	4	11.310	352003	20.0
2,6,10-Dodecatr...	14.821	4.0	ng	56909	6	15.457	288453	20.0